THORLABS

ThorSpectra

v3.39

User Guide

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Chapter 1 Software Introduction

ThorSpectra is a general spectrum analyzer software designed to be used with a number of Thorlabs instruments, such as:

- **CCTxx:** Compact CMOS spectrometer featuring trigger capability and an integrated internal shutter.
- **OSA20xC & Redstone® OSA30x**: Optical Spectrum Analyzers covering wavelength ranges from 350 nm to 12 µm with a resolution of 7.5 GHz (Item # OSA20xC) or 250 nm to 5.6 µm with a resolution of 1.9 GHz (Redstone Item # OSA30x).
- **RSB1(/M) & RASPx:** Modular Raman Spectroscopy Kit (Item # RSB1(/M)) and Compact Desktop Raman Spectrometer (Item # RASPx).
- **CCSxxx**: Legacy compact CCD spectrometer with no moving parts and up to 200 scans per second.

Many GUI features are common to all instruments while some are device-specific. This document will cover the common functionalities and the device-specific customizations are described in the respective instrument manual.

Chapter 2 Software Setup

2.1. Requirements

The minimum system requirements for running ThorSpectra depend on the device you are using. Please refer to the specifications listed below to ensure your system meets the necessary requirements.

Note: Do not connect the instrument to your PC before the software has been completely installed.

2.1.1. CCTxx Spectrometers

Minimum Hardware and Software Requirements

- Operating System: Windows® 10 or 11 (64-bit)
- Minimum Monitor Resolution: 800 x 600 pixels
- Processor: Intel Core i5 or AMD Athlon II
- 8 GB RAM
- 2 GB of Available Hard Drive Disk Space
- .NET Framework 4.7.2 or higher

For optimal performance Thorlabs suggests the following configuration:

Recommended Hardware and Software Requirements

- Operating System: Windows 11 (64-bit)

You will also need a USB cable qualified for the high-speed USB 2.0/3.0 standard (a suitable cable is included with the instrument).

2.1.2. OSA20x and Redstone® OSA30x Instruments

Minimum Hardware and Software Requirements

- Operating System: Windows® 7 SP1, 8, 10, or 11 (64-bit)
- Minimum Monitor Resolution: 800 x 600 pixels
- Processor: Intel Core i5 or AMD Athlon II
- 8 GB RAM
- .NET Framework 4.7.2 or higher

For optimal performance Thorlabs suggests the following configuration:

Recommended Hardware and Software Requirements

- Operating System: Windows 11 (64-bit)
- Processor: Intel Core i9 or AMD Athlon Ryzen
- 16 GB RAM

You will also need a USB cable qualified for the high-speed USB 2.0/3.0 standard (a suitable cable is included with the instrument).

2.1.3. RSB1(/M) and RASPx Raman Spectrometers

Minimum Hardware and Software Requirements

- Operating System: Windows® 10 or 11 (64-bit)
- Processor: Intel Pentium 4 or AMD Athlon 64 3000+
- Minimum Monitor Resolution: 800 x 600 pixels
- 2 GB RAM
- 2 GB of Available Hard Drive Disk Space
- .NET Framework Version 4.5.2 or Higher

For optimal performance Thorlabs suggests the following configuration:

Recommended Hardware and Software Requirements

- Operating System: Windows® 11 (64-bit)

You will also need a USB cable qualified for the high-speed USB 3.0 standard (a suitable cable is included with the instrument).

2.1.4. Legacy CCSxxx Spectrometers

Minimum Hardware and Software Requirements

- Operating System: Windows® 7 SP1, 8, 10, or 11 (64-bit)
- Minimum Monitor Resolution: 800 x 600 pixels
- Processor: Intel Core i5 or AMD Athlon II
- 8 GB RAM
- 2 GB of Available Hard Drive Disk Space
- .NET Framework 4.7.2 or higher

For optimal performance Thorlabs suggests the following configuration:

Recommended Hardware and Software Requirements

- Operating System: Windows 11 (64-bit)
- Processor: Intel Core i9 or AMD Athlon Ryzen
- 16 GB RAM

You will also need a USB cable qualified for the high-speed USB 2.0/3.0 standard (a suitable cable is included with the instrument).

2.2. Software Installation

If the instrument is shipped with a laptop, all required drivers and software are pre-installed. If you wish to install the software on another computer or need to re-install the software, please download the installer from Thorlabs' website:

- **CCTxx:** https://www.thorlabs.com/software-pages/cct
- **OSA20xC & Redstone® OSA30x:** https://www.thorlabs.com/software-pages/osa
- **RSB1(/M) and RASPx:** https://www.thorlabs.com/software-pages/osaraman
- **CCSxxx** (discontinued)**:** https://www.thorlabs.com/software-pages/ccs

The installation package will install all the necessary software and drivers for the instrument. A single computer can control several instrument types simply by installing the different installers after one another. A prompt may appear asking for “Elevated mode” or “Administrator mode;” please ask your system administrator if you do not have administrator privileges.

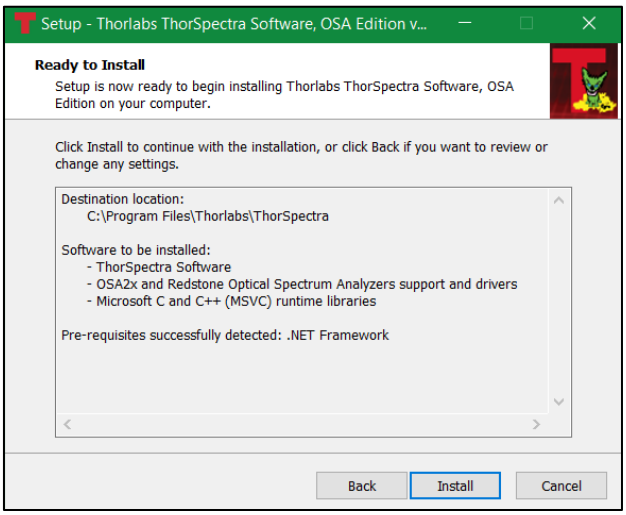


Figure 1. Software Setup Screen

2.3. Connecting to the PC

After the software installation has finished, you can connect the instrument to an available USB port on the PC. **Use only the cable that is included with the instrument**, as quality can differ between producers. When connecting a CCTxx instrument to a computer without an available USB Type-A port, a USB Type-C® port can be used with any shielded USB Type-C cable.

After connecting the instrument to the PC, the operating system will load the appropriate USB drivers. Please wait for this procedure to finish before doing anything else.

2.4. Starting the Application

After the PC software is installed and the instrument is connected to the PC, the application controlling the instrument may be started. The ThorSpectra software can be found by clicking the “Start” button and then “Thorlabs” (or “Programs” → “Thorlabs” → “ThorSpectra” depending on your Windows® version), and clicking on the application icon named “ThorSpectra.”

When the ThorSpectra application starts, it will automatically detect all compatible Thorlabs instruments connected to the PC. A list of all connected devices can be seen by clicking the button “Devices” found under Instrument in the main window menu.

Chapter 3 Operation

3.1. Interface Overview

When the ThorSpectra software is first started, the main window is composed of five areas:

- **Main Menu**: contains the command buttons
- **Settings Bar**: provides quick access to the acquisition settings of the software
- **Trace Controls**: click on the Trace Label to open the Trace Options menu
- **Data Display Area**: this area displays the data collected by the instrument
- **Status Bar**: shows information about the last acquisition

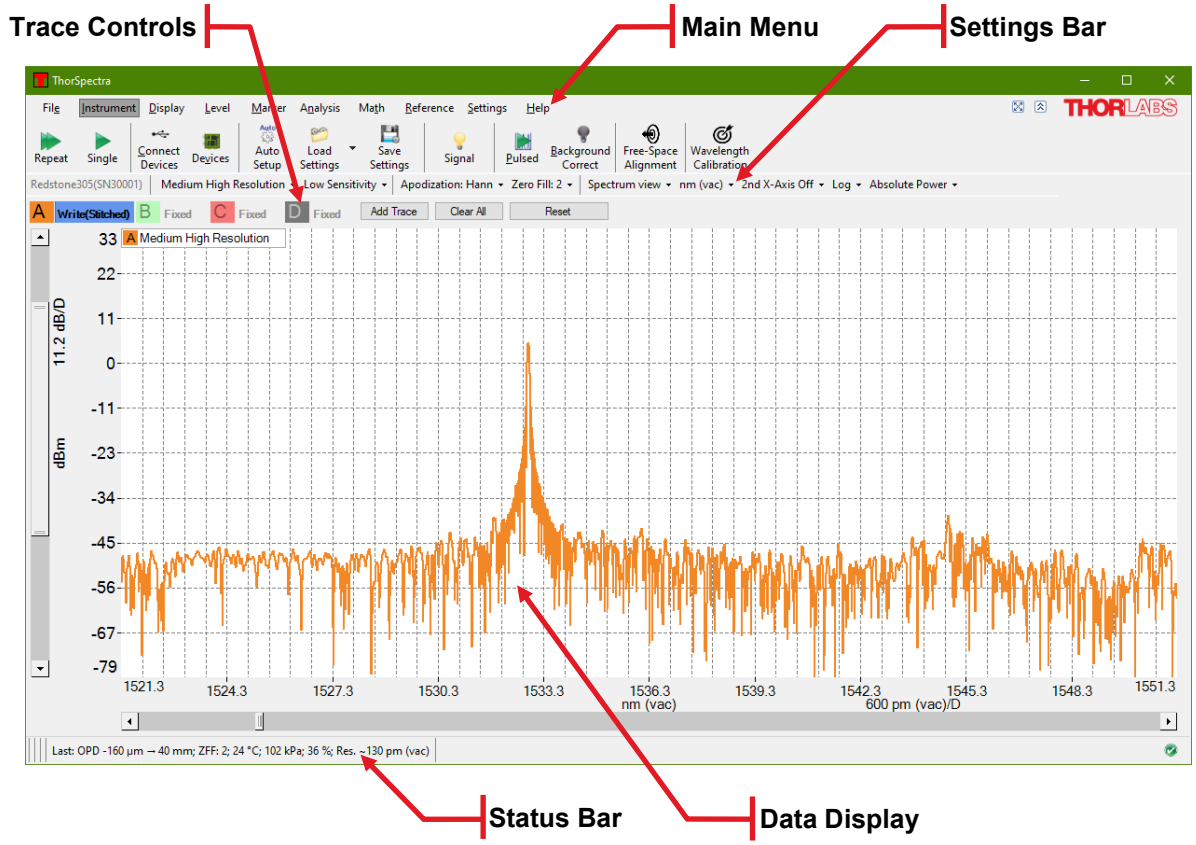


Figure 2. Layout of the Main Window of the ThorSpectra Software at Startup (when a Redstone® OSA30x Instrument is Connected)

The data display area contains a graph showing the values of the currently loaded traces. The display area is capable of showing two vertical axes: one primary axis with its unit and range shown on the left-hand side of the graph and one secondary with its unit and range shown on the right-hand side of the graph (only displayed when any trace is drawn on the secondary vertical axis). Traces can be assigned to be plotted on either vertical axis. A second horizontal axis can also be activated so that two units can be displayed simultaneously. All traces will be plotted on both these axes. In the background is a 10 by 50 grid, whose divisions are customizable by right clicking on each axis.

3.2. Customizing the Display

3.2.1. Zooming and Scrolling the Horizontal Axis

When first acquiring a spectrum or interferogram, the display is set to show the entire data range of the traces.

The data display can be zoomed in or out horizontally by:

- Scrolling the mouse wheel (hold down the Ctrl button for extra speed)
- Pressing Ctrl and “+” or “-” on the keyboard
- Changing the width of the slide bar displayed below the horizontal axis

The data display can be scrolled horizontally by:

- Dragging the data display area with the left mouse button pressed
- Simultaneously pressing Ctrl and the left or right arrow button on the keyboard
- Sliding the slide bar displayed below the horizontal axis

The horizontal display range can be set more precisely by typing in a desired minimum and maximum value in the two text boxes found under the Display menu. The horizontal display range can also be set by clicking on the horizontal axis itself, which will bring up a dialog box (see Figure 3) in which the minimum and maximum values and division, or alternatively the center value and span, can be set.

Note that the displayed horizontal range can be locked by checking the “Lock Axis” option in the dialog box displayed below. A locked axis cannot be dragged or zoomed using the mouse or keyboard in order to prevent an accidental change of the data display range.

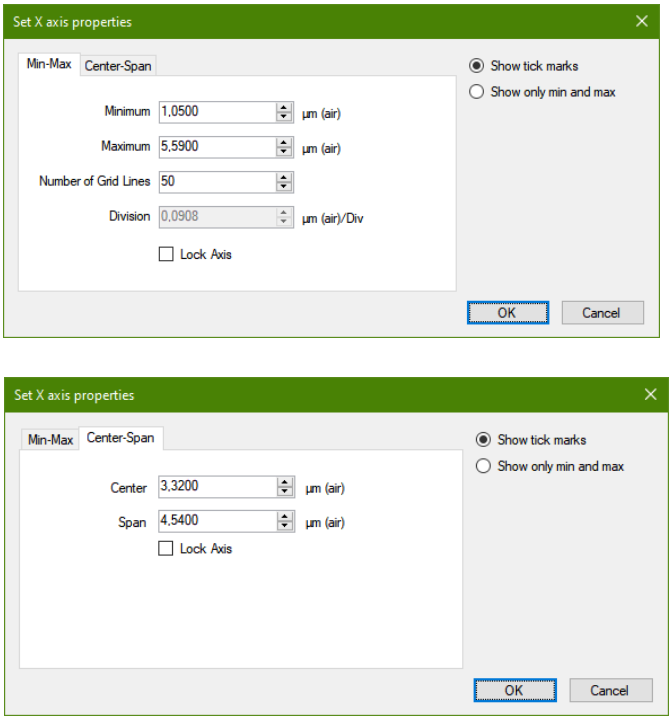


Figure 3. Axis Properties Dialog Opened for the Horizontal Axis

If two vertical line markers are displayed, the horizontal display range can also be set to the range between the two line markers by opening the Display menu and pressing the button “Get From Line Markers.”

To restore the display area to the full horizontal range, open the Display menu and click the button “Zoom Out”, or scroll the mouse wheel until the full horizontal axis is displayed.

3.2.2. Zooming and Scrolling the Vertical Axis

The primary vertical axis can be zoomed and scrolled by using the slide bar displayed to the left of the vertical axis. In the same way, the secondary vertical axis can be zoomed and scrolled using the slide bar displayed to the right on the secondary vertical axis (this axis is only visible when a trace is plotted on it).

The vertical axis can also be set manually by clicking on the (primary or secondary) vertical axis itself. This will bring up a dialog box, (similar to the one shown in Figure 3) in which the minimum and maximum values and division, or alternatively the center value and span, can be set.

Right clicking anywhere in the graph will resize the vertical axis to fit the full vertical range of the currently displayed data (as determined by the settings for the horizontal axis).

If both level markers are displayed, the vertical range can be set to the range between the level markers by opening the Level menu and clicking the button “Get From Level Markers.”

Note that the displayed vertical range of the primary and/or secondary can be locked by checking the option “Lock Axis” in the dialog box displayed above. A locked axis cannot be dragged or zoomed using the mouse or keyboard in order to prevent an accidental change of the data display range.

3.2.3. Setting the Unit of the Horizontal Axis

It is possible to change the horizontal axis unit by using the x-axis unit drop-down menu in the settings bar. The available options are:

- Wavenumber (cm^{-1})
- Raman Shift Wavenumber (cm^{-1})
- Wavelength (nm) in Air
- Wavelength (nm) in Vacuum
- Frequency (THz)
- Photon Energy (eV)

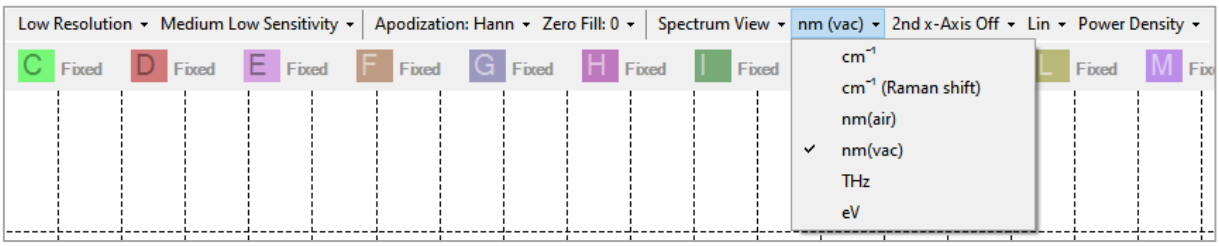


Figure 4. Setting the Horizontal Axis Unit

3.2.4. Displaying the Secondary Horizontal Axis

It is possible to add a secondary horizontal axis, simply by selecting a unit for it in the 2nd x-axis drop-down menu in the settings bar. The available options1 are the same as for the primary axis.

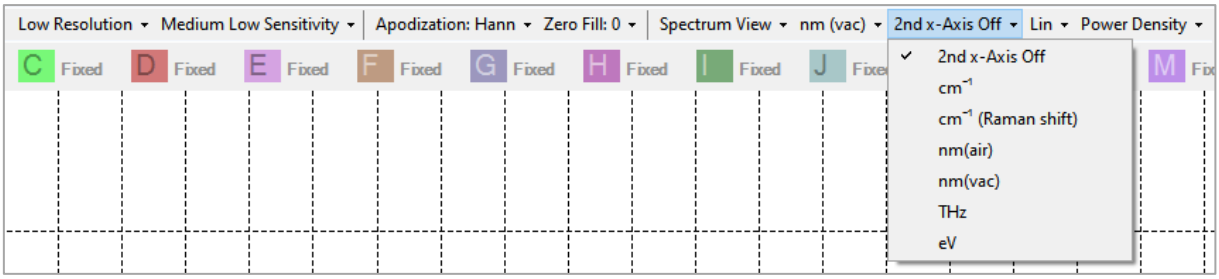


Figure 5. Showing the Secondary Horizontal Axis and Setting its Unit

3.2.5. Setting the Unit of the Vertical Axis

The vertical axis is set by default to show optical power in linear scale in mW, but it can also be set to dBm by selecting “Log” from the vertical axis unit drop-down menu in the settings bar.

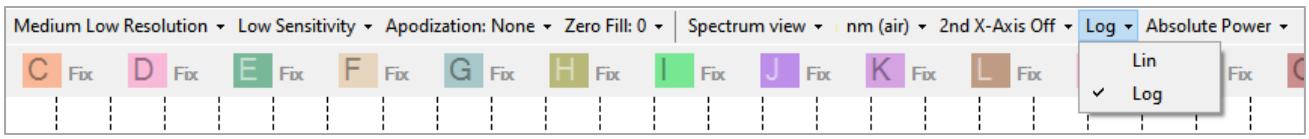


Figure 6. Setting the Vertical Axis Unit

3.2.6. Displaying the Secondary Vertical Axis

In the ThorSpectra software the traces can be shown on either the primary axis with its labels and units displayed to the left of the graph or on the secondary axis with its labels and units displayed to the right of the graph.

To change on which vertical axis a trace is displayed, click the icon of the trace you want to change. This will bring up a menu with options and operations for that trace. Click on the option “Move to secondary axis” to move the trace to the secondary axis. To move the trace back to the primary axis, click on the trace again, and the option will have changed to “Move to primary axis.” Every trace displayed on the secondary axis will have a small arrow displayed next to its icon in the Trace controls bar that looks like this:



When working with data on both the primary and secondary vertical axes:

- The range of the primary and secondary axes can be set individually by clicking on (the gray part of) the axis which brings up the Axis Properties dialog (see Figure 3) for the selected axis. Note that the grid density is always the same for the primary and the secondary axes; changing the grid density on one axis will change the grid density on the other.
- Right clicking on the graph will rescale both the primary and the secondary axes.
- The primary and secondary axes can be locked individually to any desired range by checking the “Lock Axis” check box in the corresponding Axis Properties dialog (see Figure 3).
- Changing Linear/Log mode or Absolute Power/Power Density mode will change the units of both the primary and secondary axes.

In Figure 7, Trace A (black) is shown on the primary axis while Trace B (red) is displayed on the secondary axis. Note the small arrow on the icon for Trace B showing that Trace B is displayed on the secondary axis.

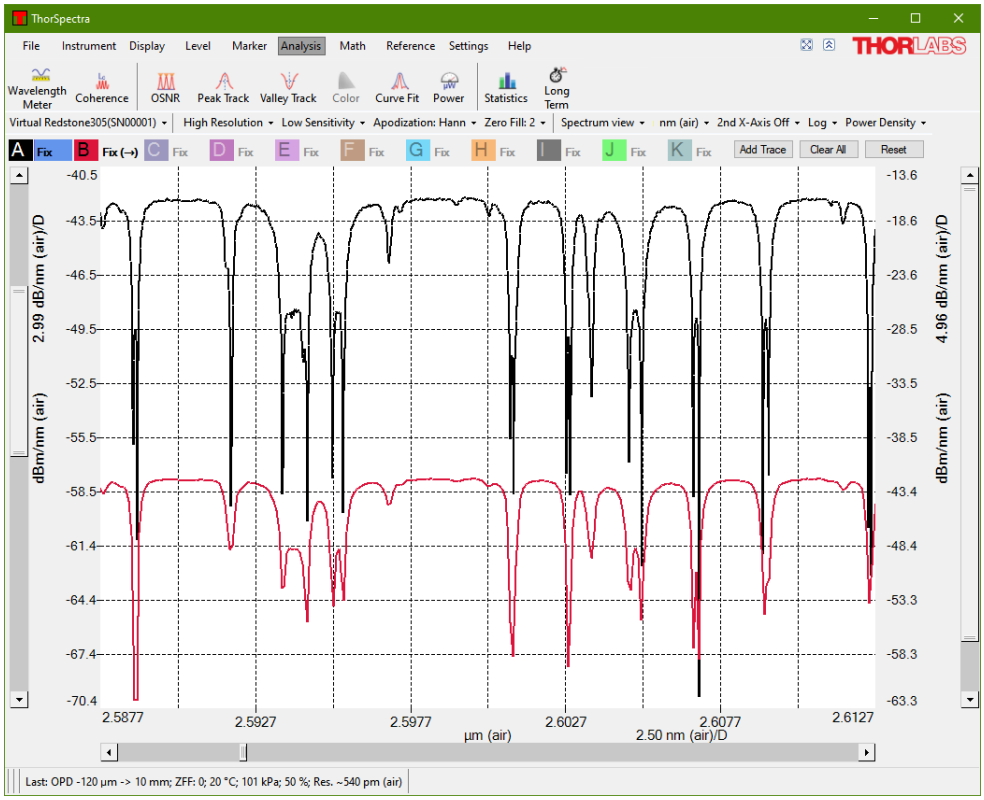


Figure 7. Displaying Data on Both the Primary and Secondary Vertical Axes

3.2.7. Hiding the Menus and Full Screen Mode

There are two buttons located in the top right corner of the main menu, close to the Thorlabs logo.

- The left button toggles between full screen mode and regular window mode.
- The right button collapses or expands the main menu. The first time this button is clicked, the main menu will collapse so that the second row is hidden completely and only the labels of the top-level menu are shown. The menu can be expanded again by pressing the same button or by clicking on any label of the top-level menu.



3.2.8. Switching Between Power Density and Absolute Power

The power per wavelength, or frequency, unit is called the power density (e.g., mW/nm or dBm/THz) and the power per resolution unit is called the absolute power. By default, ThorSpectra is set to display the retrieved spectra in Absolute Power mode. The display can be switched between Power Density and Absolute Power mode by using the drop-down menu in the settings bar (see Figure 8).

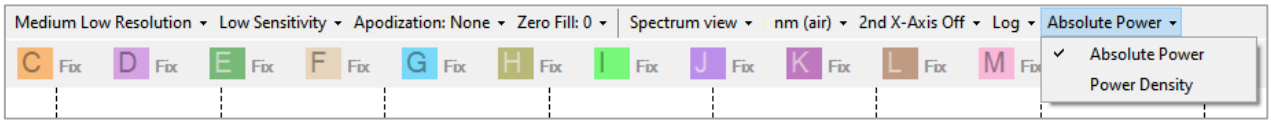


Figure 8. Switching Between Power Density and Absolute Power Mode

For light coming from a very narrowband source such as a laser, the bandwidth of the source is smaller than the resolution of the instrument and all the optical power is accommodated within one resolution unit in the measured spectrum. Thus, the peak level of the measured spectrum is equal to the total power of the light source when the display is set to Absolute Power.

For light from a broadband source such as LEDs, the bandwidth of the source is much larger than the resolution of the instrument and the level of the measured spectrum will vary with the resolution mode when the display is set to Absolute Power. By setting the display mode to Power Density, it is possible to compare spectra from broadband sources measured at different resolution modes.

- Absolute Power mode is the recommended mode for narrowband sources.
- Power Density mode is the recommended mode for broadband sources.

When the display is set to Absolute Power, the y-axis unit will display the power unit (e.g., nW or dBm). When the display is set to Power Density the y-axis unit will display the power unit per x-axis unit (e.g., nW/nm or dBm/cm^{-1}).

3.2.9. Displaying a Split View

The Display menu features a drop-down menu, with which additional data can be displayed. Selecting the option “Split View” will show a secondary display area above the main display area. The two areas show the same data, but whereas the displayed ranges in both x and y can be adjusted in the lower display, the entire data range is displayed in the upper display. The horizontal portion of the data range that is not displayed in the lower area is grayed out in the upper area.

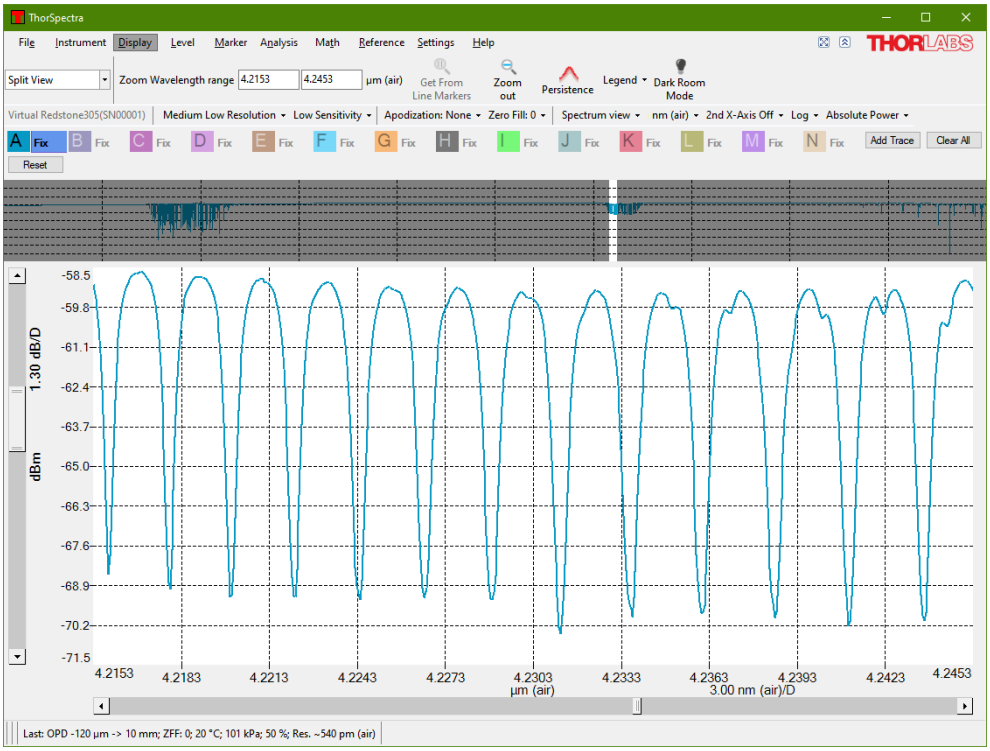


Figure 9. Split View

3.2.10. Displaying a Legend in the Data Display Area

A legend can be added to the main data display to make it easier to remember what each collected trace contains. The text in the legend can be taken from the name of the trace, from the comment of the trace, the filename of the trace (only applicable if the trace was saved or loaded from a file), or from the resolution or sensitivity setting applied when the trace was collected.

To enable the legend and choose which option determines the text, use the Display menu in the main window or the Display page in the Settings dialog (see Section 4.1 Display Settings).

If the legend text is being taken from the name of the trace or the comment of the trace, it is possible to edit the text directly in the legend. Simply double-click on the text you wish to change — it will be saved automatically when pressing the Return key. To discard the changes before they are saved, press the Escape key on the keyboard.

It is also possible to enter subscripts, superscripts, and Greek letters into the name or comment of the trace. To insert a single subscript character, type '_' (underscore) before the character that you wish to subscript (e.g., '_0' will produce a subscript zero). Superscript characters are inserted by typing '^' (caret) before the character that you wish to superscript. To insert multiple subscripted and superscripted characters, enclose the characters in curly brackets (e.g., 'SO_4^{3-}' will produce SO_4^{3-}). To insert a Greek character, type '\' (backslash) followed by the name of the letter (e.g., '\mu' will produce µ).

The name of the trace and the comment of the trace can also be modified through the Trace Info dialog, as described in Section 3.6.4 Viewing Properties of a Trace.

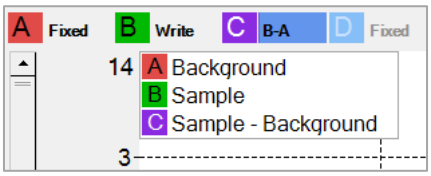


Figure 10. Displaying a Legend in the Data Display

3.2.11. Dark Room Mode

If the screen is too bright, the graph background and grid color can be easily changed by clicking the "Dark Room Mode" button under the Display menu. The background color will turn black and the grid color will turn white. Click the button again to revert the graph background color to white and grid color to black.

Certain analysis tools will be affected by the Dark Room mode. The affected analysis tools are Wavelength Meter (not available for all instruments), Coherence Length (not available for all instruments), and Power (Section 3.8.8). These analysis windows need to be opened after Dark Room mode is activated in order to be dark.

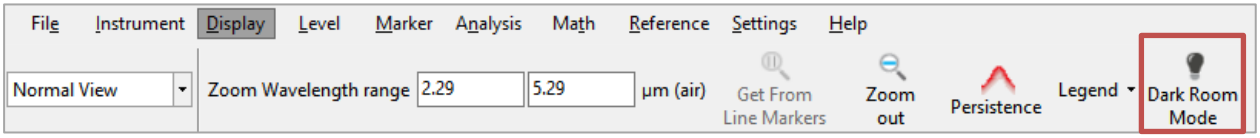


Figure 11. Dark Room Mode Button in the Display Menu

3.3. Acquiring Data

Spectra are acquired from the Active Device and processed according to the current settings.

3.3.1. Finding the Spectrometer

When the software starts it will automatically detect and read the properties of all compatible Thorlabs instruments connected to the computer through USB. If the program was started before the instrument was connected or powered-on, the software will not be able to find the instrument. To search for connected instruments, press the "Connect Devices" button found under the Instrument menu. This will cause the software to search all USB ports for connected Thorlabs instruments as well as read their properties and settings. Note that the software interface may freeze for a short while during the time in which the scan is performed. If the device cannot be found, please see Chapter 6 Troubleshooting.

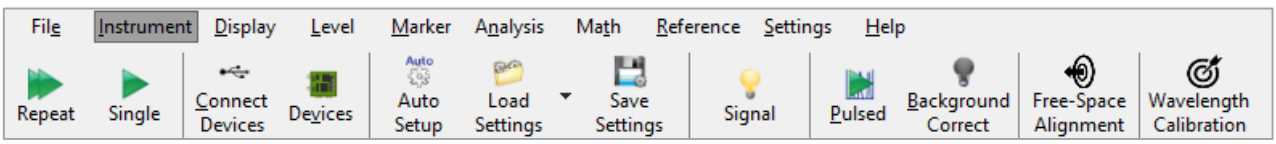


Figure 12. Instrument Menu for Redstone® OSA30x Instrument

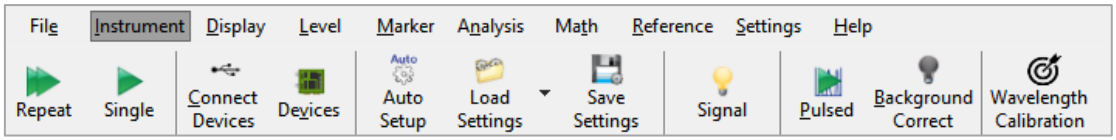


Figure 13. Instrument Menu for OSA20xC Instrument

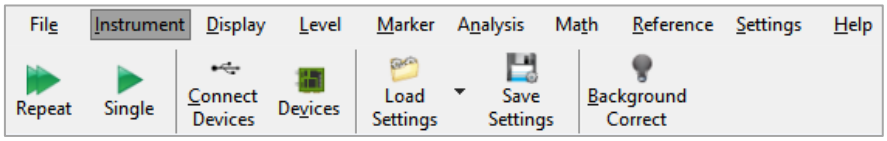


Figure 14. Instrument Menu for CCTxx, RSB1(/M), RASPx, and CCSxxx Instruments

3.3.2. Selecting with Which Instrument to Work

If several instruments are connected to the PC, the most recently connected device will be selected as the Active Device. All changes to acquisition options will be realized on that instrument and the measurement buttons “Single” and “Repeat” will control the Active Device.

The Active Device can be changed by selecting a different device from the drop-down list of devices found on the leftmost side of the screen, just above the Trace controls, see Figure 15.

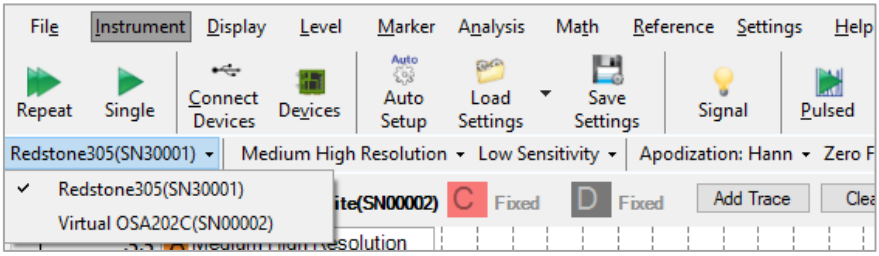


Figure 15. Selecting the Active Device from the Settings Bar

The selection can also be changed by pressing the button “Devices” found under the Instrument menu. This displays a dialog window with all currently connected devices and their properties, see Figure 16. Selecting one of the instruments and pressing the “Select” button will change from which instrument the data is collected.

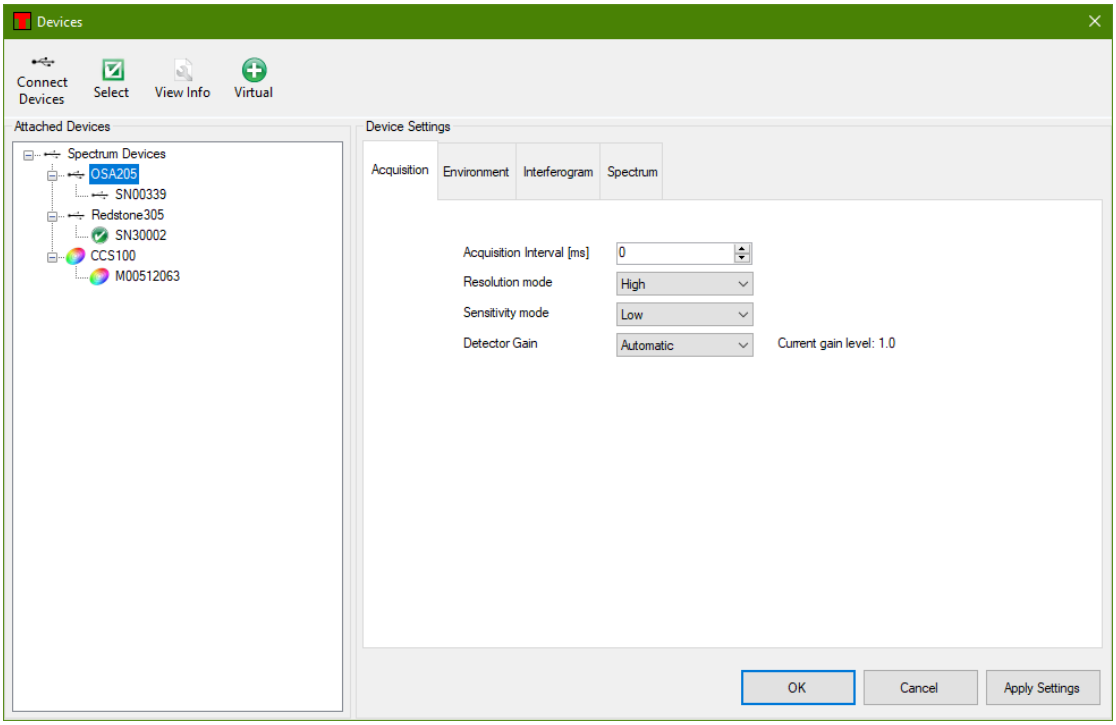


Figure 16. Devices Dialog Listing All Currently Connected Devices

To acquire data from several connected devices simultaneously, start by setting up which trace should receive data from which device. This is done in the trace menu, which is opened by clicking the Trace Icon, see Figure 20. Under the menu item “Detector,” click on the menu entry with the desired device serial number and, if applicable, channel. When the trace is setup in this way, the Trace Label displays “Write” followed by the serial number of the device. To start acquiring data from the devices, loop through selecting the devices as the Active Device and pressing “Repeat” or “Single” under the Instrument menu. Devices set to running a continuous acquisition will continue to acquire data also when another device has been selected as the Active device.

3.3.3. Acquiring a Single Spectrum

To acquire a single spectrum from the spectrometer, press the button “Single” found under the Instrument menu.

The new spectrum will be stored in the trace(s) currently in “Write” status. Note that these traces will be overwritten with the new information. Any trace set to automatic calculation will also be updated.

The Redstone® OSA30x instrument will acquire one spectrum per detector, which can be shown as a stitched spectrum or separately. Note that the noise floor of the two detectors might not be at the same level, which presents itself as a ramp in the spectrum when there is no light in the overlap region. However, the transition is power calibrated so that the two detector responses match with light input.

During the time the new spectrum is collected, the “Single” button is changed to a “Stop” button which if pressed will abort the current acquisition.

3.3.4. Repeated Measurements

To acquire multiple spectra, press the button “Repeat” found under the Instrument menu. A progress bar in the lower left corner of the window is shown and the “Repeat” button changes into a “Stop” button, signaling that the acquisition is running.

If any problem occurs during the communication with the spectrometer, a message box will appear giving information on what type of error has occurred.

As soon as new spectra are available, all traces currently in “Write” status will be overwritten with the new information. Any trace set to automatic calculation will also be updated at each acquisition.

3.3.5. Averaging Spectra

Averaging multiple spectra normally reduces noise levels of the measurement. It can therefore be beneficial to average a few spectra if the intensity of the incoming light is low.

In the ThorSpectra software, spectra are averaged as a rolling average, meaning that the screen will be updated for each new spectrum that is collected and the average of all the measured spectra will be displayed on the screen. The rolling average is calculated as

$$S_j(i) = \frac{S_{j-1}(i) \times (n-1) + S(i)}{n}, i = 1, 2, 3, \ldots, N$$

Where $S_j(i)$ is the newly displayed average, $S_{j-1}(i)$ is the previously displayed average, $S(i)$ is the newly acquired spectrum, i is the index of a data point, N is the number of data points, and n is the number of spectra to average (or, if smaller, the number of spectra averaged so far). To restart the averaging procedure, click on the trace menu option “Clear” for the trace containing the averaged spectrum; this will reset the number of spectra averaged so far (n) and the displayed average to zero.

It is possible to automatically stop the averaging when the required number of spectra have been reached by selecting one of the options in the “Average and Stop” sub-menu on the Trace Options menu (see Section 3.6 Working with Data in Traces).

3.4. Movable Markers

The ThorSpectra software has four movable markers (two line markers and two level markers), which can be enabled and disabled by pressing the respective button found under the Marker menu. The line markers are labeled “Marker 1” and “Marker 2”, and the level markers are labeled “Marker 3” and “Marker 4.” The markers can also be enabled and disabled by pressing Ctrl and their respective number on the keyboard.

The movable markers can be used to inspect the value of the data at different positions, change the displayed area of the graph (see Sections 3.2.1 and 3.2.2), or place fixed markers.

3.4.1. Moving Markers

The movable markers can be moved by placing the mouse cursor over the marker, where the mouse cursor changes into a double arrow. Press and hold the left mouse button to drag the movable marker to the desired position.

The position of the movable markers can also be changed by clicking on the number of the marker to move in the Movable Markers dialog box. This brings up another dialog in which it is possible to type in the position of the cursor manually either absolutely or relative to the other marker.

3.4.2. Marker Values

As long as any movable marker is enabled, the Movable Markers dialog box will be shown either as a floating window or docked to the main window. The dialog box shows the position of each enabled line marker, the value of the active trace at the position of the line marker(s), and the level of each enabled level marker. If both line markers are enabled, the distance between them and the difference or quotient in value of the Active Trace at the two positions is shown. If both level markers are enabled, the difference or quotient between them will be displayed. Which value to be shown can be changed by clicking the Settings icon displayed above the marker values.

3.4.3. Locking the Markers

If both level markers or both line markers are displayed, a small padlock is displayed just to the left of the difference/quotient label. Clicking this padlock will lock the relation of the markers, so that moving one of the markers will also move the other by the same amount. Whenever two markers are locked, a locked padlock will be displayed; clicking this padlock again will unlock the markers.

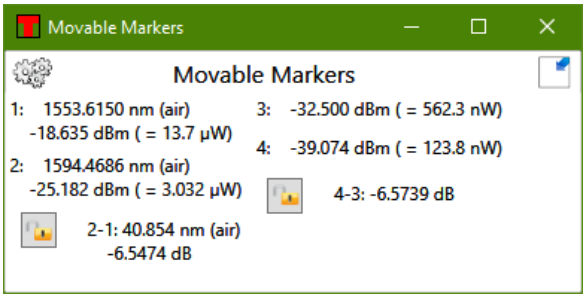


Figure 17. Movable Markers Dialog Box

3.5. Fixed Markers

The ThorSpectra software can handle up to 2048 fixed markers. A fixed marker has a fixed horizontal position and is connected to a single trace (not necessarily the Active Trace) and will track the value of its trace at the given position. Fixed markers are identified by a number, and the levels of the fixed markers can be tracked in a Long-Term analysis.

Each fixed marker added is shown in the data plot as a triangle with its identifying number above it. The location of the triangle is determined by the position of the fixed marker and the value of the connected trace at the given position.

The values of the fixed markers and their positions can be stored to file or copied to the clipboard for processing in another software.

3.5.1. Adding Fixed Markers

A fixed marker can be added to the currently active trace by moving line Marker 1 to the desired position in the data plot and pressing the button “Add Fixed” found in the right part of the Marker menu (see Figure 18). The fixed marker can be removed by moving line Marker 1 to the approximate position of the fixed marker to remove and pressing the button “Remove Fixed,” or alternatively by right-clicking the fixed marker in the data table and selecting “Remove Marker.”

3.5.2. Moving Fixed Markers

A fixed marker can be moved to a specific position by typing a new number into the Position column in the data table, see Figure 19.

3.5.3. Automatically Mark Peaks

Pressing the button “Mark Peaks” will add one fixed marker to each peak in the currently Active Trace that has previously been automatically detected with the Peak track analysis tool (see Section 3.8.4 Peak Track). The first marker will be added to the highest peak in the spectrum, the second marker to the second highest peak, etc. Note that this will add fixed markers to the found peaks in the currently Active Trace; the positions of these markers will not change until you move them.

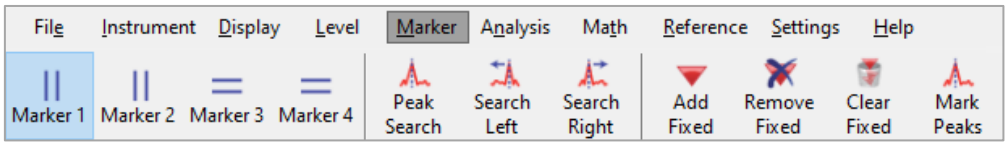


Figure 18. Marker Menu

3.5.4. Value of Markers

As long as at least one fixed marker is enabled, a data table will be shown in the area below the main data display area (see Figure 19) or in a separate floating window. The data table lists all currently shown fixed markers with its identifying number, the trace to which the fixed marker is connected, position, and the value of the connected trace at the fixed marker’s position. Further data columns are also displayed, such as “ΔPosition” (relative position of the marker to the preceding marker, in current x-axis units), “Offset” (relative position of the marker to the first marker, in current x-axis units), and “ΔLevel” (relative level of the Active Trace at the marker

to the preceding marker, in current y-axis units). Right-clicking in the data table will bring up a context menu through which it is possible to bring a marker into view or remove it, copy a line or the entire table to the clipboard, or save the data table to file. A fixed marker can be moved by editing the value in the position column.

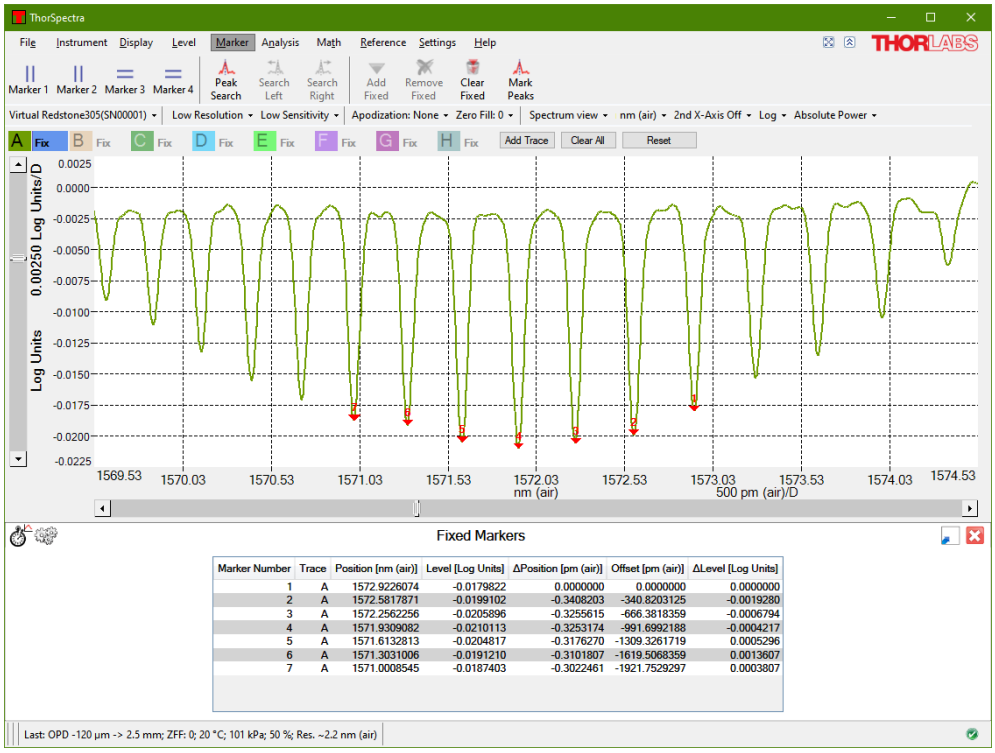


Figure 19. Fixed Marker Data Table Shown Below Main Data Display Area

3.6. Working with Data in Traces

The collected spectra are stored in what are called “traces.” The ThorSpectra software can handle up to 26 traces labeled from A to Z for spectra. The controls for the traces are found in the area between the data display area and the main menu (see Figure 2). The color of each trace in the data display area corresponds to the square surrounding the Trace Icon in the trace control area; traces which are not currently displayed in the data display area are shown in colors with less saturation than the displayed traces.

3.6.1. Active Trace

One of the traces will be marked as the Active Trace. This is indicated by the blue background of the Trace Label, just to the right of the Trace Icon (“A”, “B”, etc.). The Active Trace is the trace onto which all math operations are applied, the trace that is analyzed by the analysis tools, and the trace that is saved when the “Save trace” menu item is selected. To designate a trace the active status, click on the Trace Label to open the Trace Options menu and select “Set as Active.”

3.6.2. Trace Update Options

The Trace Label to the right of the Trace Icon displays the update option for the trace. This option determines what will happen with the trace during the next data acquisition. To change the update option for a trace, click on the Trace Label to bring up a menu with options and operations for the trace. The top line of the menu displays the name of the trace. To move a displayed trace from the primary axis to the secondary axis, click on the option “Move to secondary axis.” To move the trace back to the primary axis, click on the trace again; the option will now have changed to “Move to primary axis.” The secondary axis in the data display area will only be shown if at least one trace is drawn on it.

The following standard update options are available:

- **Write**: Traces with this option will be overwritten at the next acquisition. If multiple devices are present, the option exists to specify the device with which to update the data. For devices with multiple detectors, it is also possible to select to view data from one of the detectors or a stitched combination thereof.

- **Fix**: Traces with this option will not be updated at the next acquisition.

- **Average**: Traces with this option will be updated at the next acquisition as a rolling average of the data already existing in the trace and the newly acquired data. It is possible to have the running average stop updating once the desired number of spectra has been collected by selecting the option “Average and Fix.” The Trace Label will show how many spectra have been collected thus far, e.g., “Avg(1 of 5).”

- **Min Hold**: Traces with this option will be updated as the minimum of the currently existing data in each data point in the trace and the newly acquired spectrum from the selected detector.

- **Max Hold**: Traces with this option will be updated as the maximum of the currently existing data in each data point in the trace and the newly acquired spectrum from the selected detector.

- **Difference**: Traces with this option will be updated as the difference between two other traces *to the left* in the Trace controls bar. The Trace Label will signify how the trace will be calculated, e.g., “B-A” or “A-C.” This trace will be updated when any of the traces involved in its calculation are updated. This option is available under the Calculate sub-menu for traces with at least two traces to the left, e.g., this option is available for traces C and higher.

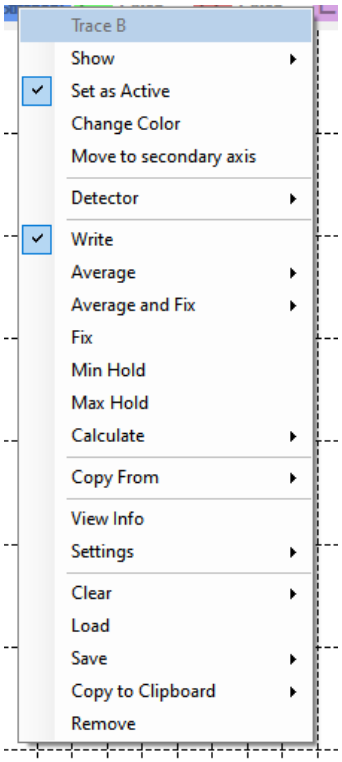


Figure 20. Trace Options Menu

- **Quotient**: Traces with this option will be updated as the quotient between two other traces *to the left* in the Trace controls bar. The Trace Label will signify how the trace will be calculated, e.g., “B/A” or “A/C.” This trace will be updated when any of the traces involved in its calculation are updated. This option is available under the Calculate sub-menu for traces with at least two traces to the left, e.g., this option is available for traces C and higher.

- **Transmission**: Traces with this option will be updated as a quotient between two other traces *to the left* in the Trace controls bar, expressed in percent. The Trace Label will signify how the trace will be calculated, e.g., “Transmission(B, A)” which will calculate B/A. This trace will be updated when any of the traces involved in its calculation are updated. This option is available under the Calculate sub-menu for traces with at least two traces to the left, e.g., this option is available for traces C and higher.

- **Absorbance**: Traces with this option will be updated as $-\log_{10}(T_1/T_2)$ where T_1 and T_2 represent two separate traces *to the left* in the Trace controls bar. The Trace Label will signify how the trace will be calculated, e.g., “Absorbance(B, A).” This trace will be updated when any of the traces involved in its calculation are updated. This option is available under the Calculate sub-menu for traces with at least two traces to the left, e.g., this option is available for traces C and higher.

- **Derivative**: Traces with this option will be updated as the derivative of another trace *to the left* in the Trace controls bar. The Trace Label will signify in an abbreviated form how the trace will be calculated, e.g., “Derivative(A, 1)” or “Derivative_FD(C, 3),” where the letters A and C are of which trace the derivative is calculated, the numbers one and three stand for the derivative order, and “Derivative” and “Derivative_FD” signify the derivative method to use; Savitsky-Golay or Finite difference, respectively. This trace will be updated when the input trace is updated. This option is available under the Calculate sub-menu, for all traces except the left-most, i.e., this option is not available for trace A.

If the calculation of a trace cannot be performed, e.g., if the two input traces have different lengths, the Trace Label background will be red and the reason for the error will be displayed in a popup when hovering over the Trace Label with the mouse pointer.

3.6.3. User-Defined Update Options

In addition to the pre-configured update options, it is possible to use an expression defined by the user. This can be reached by selecting the menu item “Calculate”→”User Defined” in the Trace Options menu. This opens

a dialog with a text box where it is possible to enter an expression to be calculated upon each acquired spectrum, using the following rules for formatting:

- Spectrum traces are identified by letters A through Z (case insensitive). Only the traces which can be seen in the Trace controls area can be used.
- Use a decimal point (full stop, '.') as decimal mark.
- Allowed operators are: subtraction ('**-**'), addition ('**+**'), division ('*/*'), multiplication ('*****') and power of ('**^**').
- Operations can be grouped or nested using round parentheses.

The expression can also contain mathematical functions. These are listed and inserted by clicking on the button labelled "Fx." Numerical values are evaluated in linear (mW) space, so that "A+5" is interpreted by the calculator as "add 5 mW to trace A."

Examples of possible update options are:

- A+B
- Exp(-A*B)
- -Log10(A/B)
- MinHold(A-B)

3.6.4. Viewing Properties of a Trace

To see the properties of a trace, click on the icon or the label of the trace that you want to inspect, and select the menu item "View Info." This will open a window displaying basic information of the trace, such as the serial number of the device, date and time of the acquisition, and the settings that were used during the acquisition.

The Trace info window will hover above all other windows as long as it is open and automatically update whenever the trace is updated.

The Trace info window contains two editable input fields named "Name" and "Comment."

- The Name field allows the user to give the trace a short name. The name can be up to 32 characters long. The name will be stored when saving the trace to file.
- The Comment field allows the user to give a longer description of the trace. The comment can be up to 4096 characters long. The comment will be stored when saving the trace to file.

The name and comment will be stored automatically while typing and retained when the trace is updated. Clearing the trace will only erase the data, but keep the name and comment. The name or comment can be shown in the legend of the main data display area, see Section 3.2.10 Displaying a Legend in the Data Display Area.

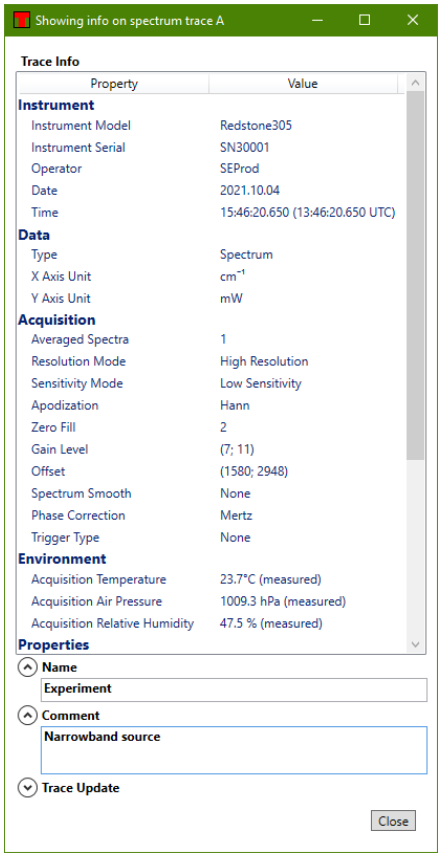


Figure 21. Viewing Properties of a Trace

3.6.5. Reordering Traces

The traces will always be drawn from the left to the right, i.e., Trace A will always be drawn first followed by Trace B, Trace C etc. If one trace covers another you may wish to change the order of the traces. This can be done by dragging and dropping the Trace Labels into the desired order. Put the mouse cursor over the icon of the trace you want to change, press and hold the left mouse button, and move the

mouse cursor to the right or the left. As you move the mouse cursor, the traces will be reordered in the Trace controls bar and in the graph. Release the left mouse button when you are content with the new order of the traces.

3.6.6. Math Operations

The Math menu includes several common mathematical operations that can be applied on traces of certain types, depending on the operation. Some buttons are not enabled in all Views or are not visible for some instruments. The buttons' functions are explained below.

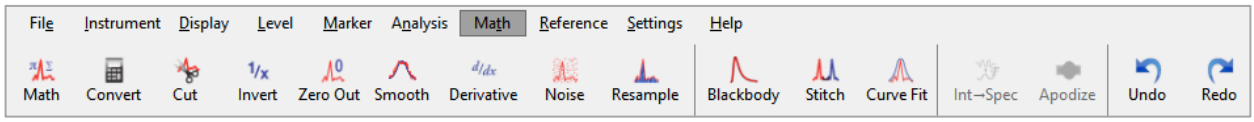


Figure 22. Math Menu in Spectrum View (for an Interferogram Device)

Math: This button brings up a dialog box (shown in Figure 23) that allows mathematical operations to be performed on one or several traces. For example, the user may multiply a spectrum by a scalar, add two spectra together, or divide one spectrum by another. The expression to be calculated is typed into the dialog box, which uses the following rules for formatting:

- Spectrum traces are identified by letters A through Z (case insensitive). Only the traces which can be seen in the trace controls bar can be used.
- Use a decimal point (full stop, '.') as decimal mark.
- Allowed operators are: subtraction ('**-**'), addition ('**+**'), division ('*/*'), multiplication ('*****') and power of ('**^**').
- Operations can be grouped or nested using round parentheses.

The expression can also contain mathematical functions; available functions are listed and inserted by clicking on the button labelled "Fx."

The calculation will be performed when the "Calculate" button is clicked or by pressing "Enter" on the keyboard. If the result of the calculation is a trace, it will be stored in the trace indicated by the drop-down menu in the dialog box. If the result of the calculation is a scalar, the calculated result will be displayed in the Result section of the dialog and it will not be saved in a trace.

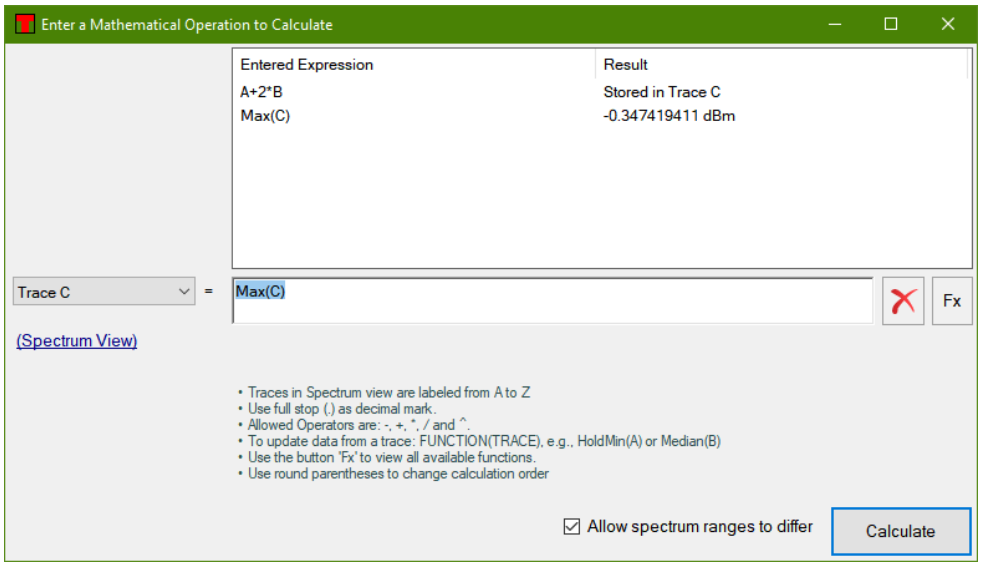


Figure 23. Mathematical Operations Dialog

Convert: Opens a small calculator where the different units used in the software can be converted to each other. Also allows for converting resolutions from one unit to another.

Cut: Cuts a trace to a specified horizontal region, removing all data outside of that region. A dialog box will open, in which the exact region and the input/output traces can be specified.

Invert: Calculates the reciprocal of the Active Trace.

Zero Out: Sets all values in a specified region of a trace to zero. A dialog box will open, in which the exact region and the input/output traces can be specified.

Smooth: Performs a smoothing operation on a trace or a region thereof. A dialog box will open, in which it is possible to select the smoothing algorithm to use and to set the parameters for the smoothing as well as the input/output traces.

Derivative: Calculates the derivative of a trace. A dialog box will open, in which the derivative order, method, and input/output traces can be specified. Derivatives are available up to the fifth order.

Noise: Adds white noise to the Active trace. A dialog box will open, in which the strength of the noise can be specified.

Resample: Changes the sample points in the Active Trace. A dialog box will open, in which it is possible to select the resampling method between a factor, copy from another trace, or every n:th data point. The resampling factor is the desired length of the trace divided by the current length of the trace. For example, selecting a resampling factor of 0.5 reduces the length of the trace by a factor of two and a resampling factor of 4.0 increases the length of the trace by a factor of four. The resampling is performed using a quintic spline interpolation to make the resampled trace as similar to the original trace as possible.

The following buttons are available only in Spectrum View:

Blackbody: Creates a spectrum from an ideal blackbody emitter. The temperature of the emitter and the horizontal range of the spectrum can be defined in the dialog that is opened. This button is only enabled in Spectrum view.

Stitch: Takes two spectra and merges them into one spectrum. The data in any overlapping region can be averaged or kept. A dialog box will be opened, in which it is possible to select the overlapping mechanism as well as the input/output traces.

Curve Fit: Fits a mathematical curve to a trace or a region thereof. A dialog box will open, in which the fit settings and input/output traces can be specified. Available math functions are: Gaussian, Lorentzian, and polynomial, see Section 3.6.7 Functional Traces (Traces Defined by a Function).

The following buttons are available only in Interferogram View:

Int→Spec: Converts an interferogram to a spectrum. Opens a dialog in which various settings can be selected.

Apodize: Performs an apodization of an interferogram. A dialog box will open, in which the type of apodization function and the input/output traces can be specified.

The following buttons are available only after a math operation has been applied:

Undo: Undoes the most recent math operation.

Redo: Redoes the most recent undone math operation.

3.6.7. Functional Traces (Traces Defined by a Function)

By using the function “Curve Fit” found under the Math menu it is possible to fit a mathematical function to a trace. The calculated function will be stored in one of the traces as a mathematical function and drawn in the data display area along with the other traces. The currently available types of functions are Gaussian, Lorentzian, and polynomial. In the dialog which is opened when pressing the “Curve Fit” button it is possible to

select the type of function to fit, the data range to use for fitting and the trace which will hold the fitted curve. If the fit failed, the status bar will display the error message “Fit Failed.”

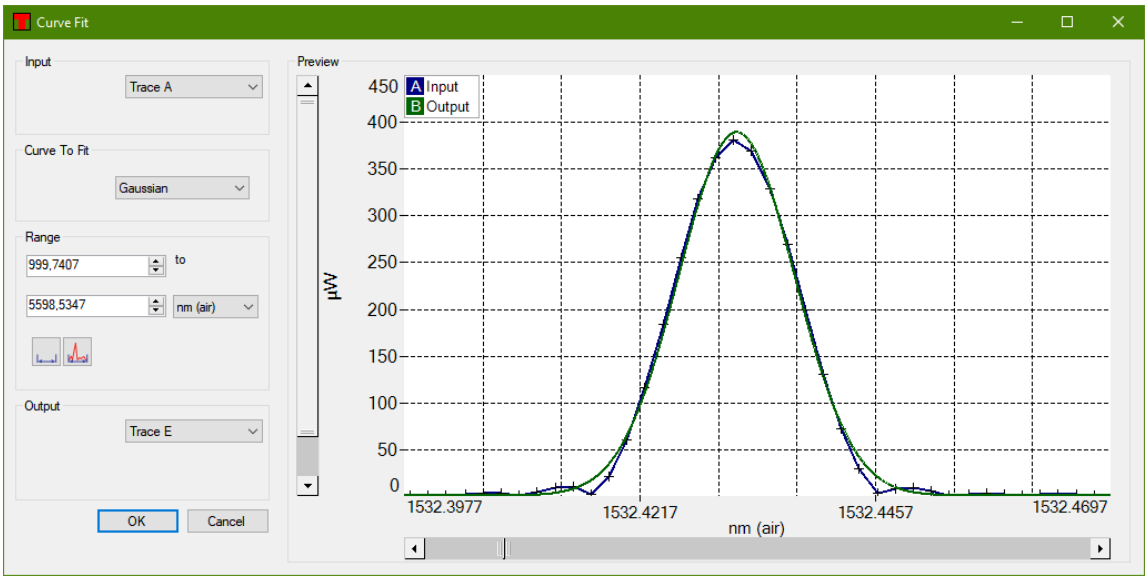


Figure 24. Curve Fit Dialog

Note that the fitted function will only be defined for the x-axis range that was used to create the function.

Opening up the trace properties window of a functional trace will display the type of function stored in the trace together with the parameter values used to define the function. Functional traces have some limitations compared to ordinary traces, not all mathematical operations can be performed on them.

3.7. Saving and Loading Data

The ThorSpectra software can read and write the following spectral file formats:

- **ThorSpectra Spectrum file format (.spf2 / .spf2x):** Native file format for ThorSpectra. Version 2.90 and older can only save and load .spf2 files whereas version 3.05 and newer can handle both .spf2 and .spf2x files.

- **Comma separated values (.csv) with ThorSpectra header:** Raw ASCII file format with a header including information about the trace and acquisition settings. Columns separated by comma, semicolon, or tab (configurable).

The software can also export spectral data in the following file formats:

- **Grams Galactic SPC (.spc):** For data exchange with other spectral software.

- **JCAMP-DX (.jdx):** For data exchange with other spectral software.

- **Matlab v5 binary file (.mat):** For easily loading data into Matlab™ and compatible software.

- **Text file (.txt):** Raw ASCII file format; columns separated by comma, semicolon, or tab (configurable).

- **Zipped text file (.txt.zip):** One txt file stored compressed in a zip folder, reduces disk usage.

- **Zipped comma separated values file (.csv.zip):** One CSV file stored compressed in a zip folder.

In the References dialog, line-by-line references with the .par file extension saved in HITRAN's 160-character format can be imported, see Section 3.9 References.

3.7.1. Saving Data

To save the data in the Active Trace, click the button “Save Trace” found under the File menu or select the menu item “Save Only this Trace” found in the Trace Options menu.

To export the data in the Active trace, click the button “Export Trace” found under the File menu.

To save the data in all traces, click the button “Save All” found under the File menu or select the menu item “Save All Traces” found in the Trace Options menu. This only allows the data to be stored in ThorSpectra Spectrum File format (.spf2 / .spf2x) or as raw data in ASCII file format, but in the latter case the files cannot be read by the ThorSpectra software.

The “Save All Visible” option, which is also available in the Trace Options menu, saves all traces with data that are not hidden. To show or hide traces, click on the Trace Label and select an option from the “Show” sub-menu.

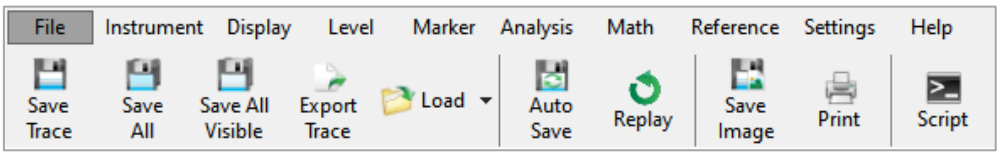


Figure 25. File Menu

3.7.2. Loading Data

There are three ways of loading spectral data into a trace.

- Click a Trace Label and select the menu option “Load” in the drop-down menu that appears. This loads the data into the selected trace, if the trace already contains data, the previous data will be erased.
- Click on the menu item “Load” found under the File menu. This loads data into the first trace that does not contain any data already. If no trace is empty, an error message will appear.
- Drag a supported file from File Explorer or another Windows® program and drop it into the main display area.

When loading files with more than one stored trace, and one or more of the stored traces are to be loaded into non-empty slot or slots, a dialog box will appear with the option to either overwrite any existing data, load the stored traces into empty slots, or to cancel the loading process and not load any trace.

3.7.3. Automatically Saving Data

ThorSpectra comes with the ability to automatically save all spectra to file as they are collected. It is also possible to store the contents of a specific trace to file in every update.

The automatic save feature is enabled and configured by clicking “AutoSave” in the File menu. This brings up the dialog displayed below.

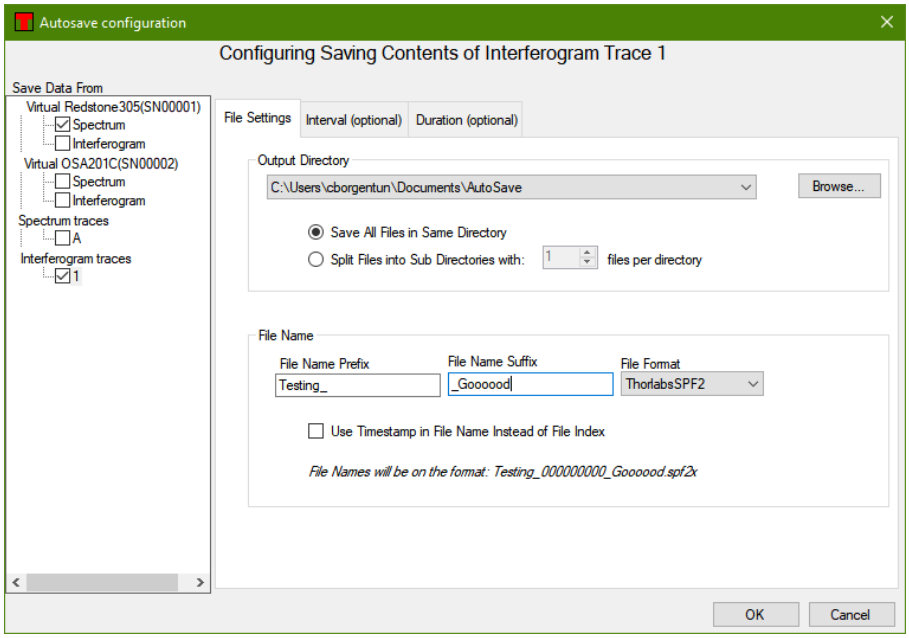


Figure 26. Setting Up Automatic Saving of Traces

Follow the steps below to enable automatic data saving:

1. In the tree view to the left, check the box next to the type of data you wish to save.
2. Select a directory in which to store the files by clicking the “Browse” button.
3. Click “Ok” to begin saving.

If the “Save All Files in the Same Directory” radio button is selected, all produced files will be stored in the selected directory. On the other hand, if the “Split Files into Sub Directories” radio is selected and a number of trace files to save in each subdirectory is specified (say, 1000), then subdirectories will be created in the specified directory, with the first subdirectory being given the name “00000.” Traces will then be saved in this subdirectory until 1000 files has been reached. A new subdirectory will be created, given the name “00001”, and used as the destination directory for the next 1000 trace files, and so on.

If the check box labeled “Use Timestamp in File Name Instead of File Index” is checked, the file name of the saved spectrum files will contain the date and time that the spectrum was collected, down to the millisecond. If this check box is unchecked, the file names will instead contain a nine-digit number which will automatically increment with each saved file.

It is also possible to specify a common prefix and suffix for the files to be saved; the names of the saved files will then be of the format:

PREFIXxxxxxxxxxSUFFIX.FILEENDING

where “xxxxxxxxx” corresponds to the nine-digit auto-incrementing number (or timestamp if that option is selected) and FILEENDING is the default file ending for the selected file format.

The second tab of the dialog box configures time limits on the automatic saving. The software can be configured to save every recorded trace, or it can save one trace per user-defined time interval. In either case, the saving can also be stopped after a time duration specified by the operating system’s clock, as configured in the third tab.

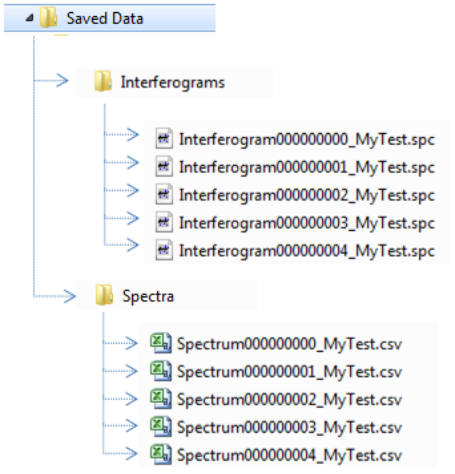


Figure 27. The Resulting File Structure When Running a Series of Measurements with Automatic Save Activated

3.7.4. Replaying Automatically Saved Data

The software can recognize data saved by the Autosave feature and replay the measurements at a later date. Click the “Replay” button in the File menu to bring up the Replay Autosaved Data dialog and click the “Change Directory” button to select a directory containing data files saved by the Autosave feature. The software will search for autosaved files and fill in the Prefix, Suffix, and Path of the found files. The measurements can then be replayed by clicking the “Play” button to play the entire set of files, or the “Skip ahead” button to show measurements one by one.

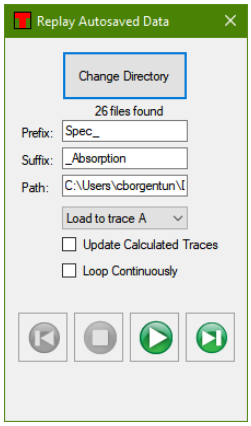


Figure 28. Replay Autosaved Data

3.8. Analyzing Data

The ThorSpectra software contains a number of analysis tools, each of which analyzes one aspect of the data from the spectrometer. The result of each analysis is displayed in a panel below the main data display area, or in a separate floating window. When an analysis tool is active, the corresponding button in the Analysis menu will be highlighted. To stop the analysis, click the corresponding button again or click the close button in the corresponding analysis window.

Some analysis tools have an options panel to the left of the displayed values. In this panel, the settings for the analysis can be seen and modified.

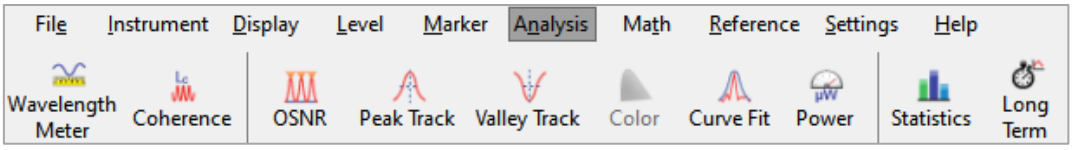


Figure 29. Analysis menu. Not all analysis tools are available for all instrument types.

3.8.1. Floating Windows

Analysis results that do not contain large amounts of data (and therefore do not require much space) are shown in a floating window above the upper-right part of the main data display area (see Figure 30). The floating window can be rescaled and moved. If the window is shrunk, some of the data will be hidden; enlarging the window makes the data reappear. The floating window can also be docked below the graph by clicking the docking button, which has a down arrow and is marked in Figure 30.

Analysis results that require more space will be docked by default. They can be moved into a floating window by clicking the undocking button, which has an up arrow and is marked in Figure 30.

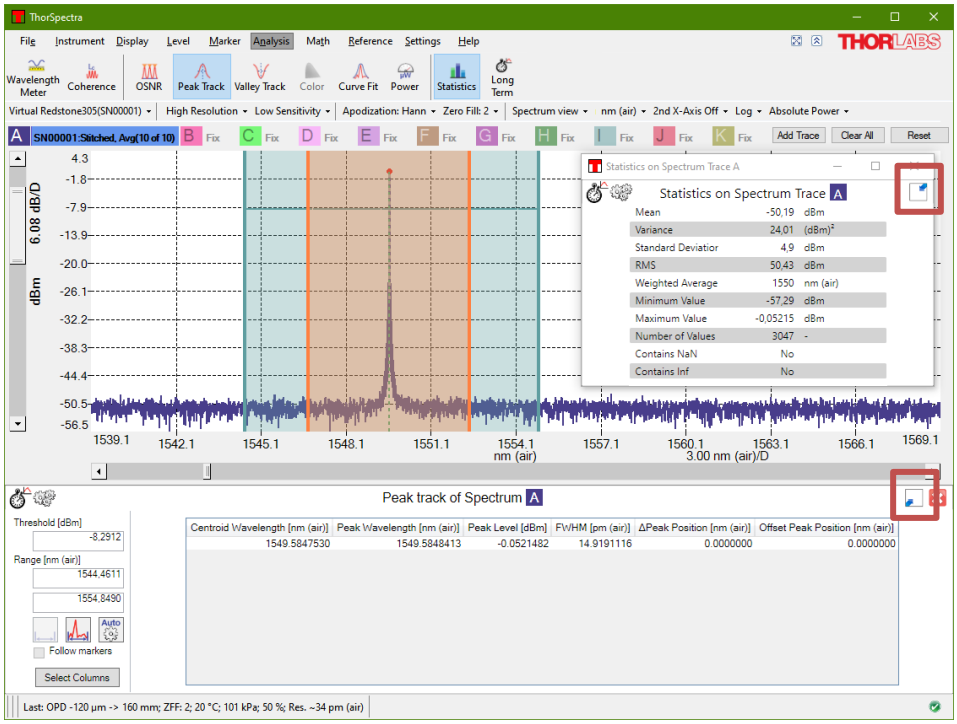


Figure 30. Analysis Displayed Beneath the Main Data Display Area and in a Floating Window

3.8.2. Displayed Range and Threshold

In some analysis tools, it is desirable to constrain the analysis to a certain portion of the trace. For these tools, a range and/or a threshold can be defined. The range and/or threshold are displayed as lines directly in the main data display, making it easy to see the part of the input signal being analyzed. The analysis range can be modified either by dragging the lines or by typing new values into the boxes in the analysis window.

If the range and threshold lines are not wanted, they can be removed from the graph by unchecking “Display Analysis Region in graph” in the analysis settings window, which is opened by clicking on the small cogwheels icon in the upper left corner of the analysis window, see Figure 31. The analysis settings window also allows the fill color of the analysis region to be changed and the fill to be disabled entirely.

By pressing the “Auto” button in the analysis window, the range and/or threshold will be set to values that are automatically determined from the displayed range of the main data display area.

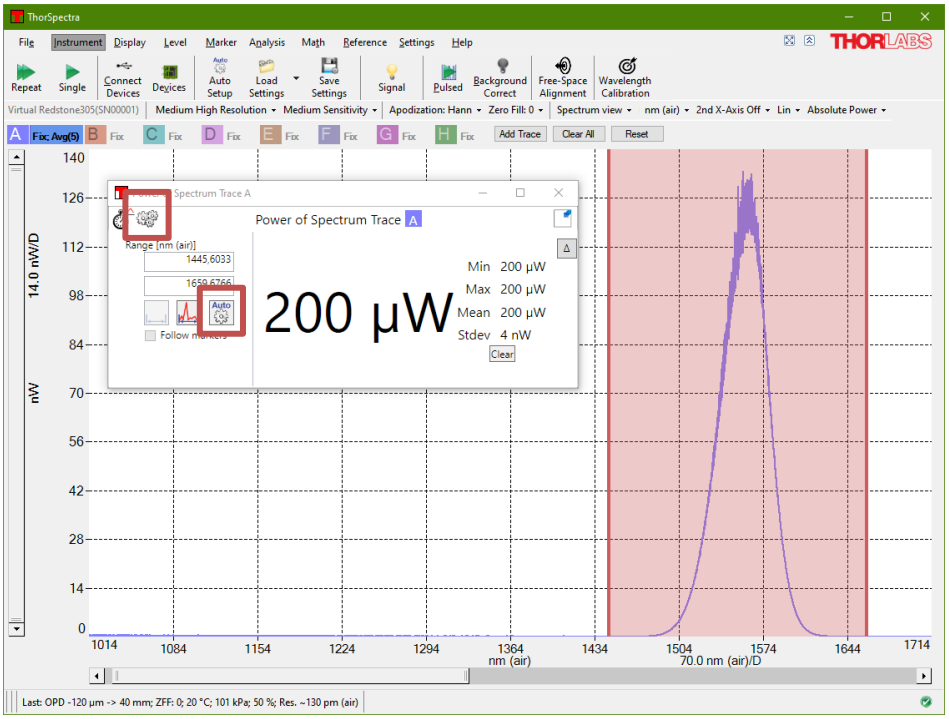


Figure 31. Power Analysis Tool with Enabled Range Lines and Fill

3.8.3. OSNR Analysis

This tool analyzes the Optical Signal-to-Noise Ratio (OSNR) of the Active Trace. It uses the parameters of the Peak Track tool to automatically find the peaks in the spectrum (see Section 3.8.4 Peak Track).

The OSNR for each peak is calculated as:

$$OSNR = 10log_{10}\left(\frac{P}{N}\right) + 10log_{10}\left(\frac{B_m}{B_r}\right)$$

Here,

- P is the optical power of the peak
- N is the interpolated noise at the peak
- B_m is the optical resolution of the measurement
- B_r is the reference resolution (0.1 nm)

When multiple peaks are present in the spectrum, the noise at each peak is calculated by the following process. First, the midpoints between the current peak and the neighboring peaks are found (note that these peaks may not be equidistant). Next, the average intensity around the left midpoint and around the right midpoint is calculated. These are the so-called left and right noise areas. Finally, the noise at the peak is linearly interpolated based upon these two values and their distance from the current peak.

For the first and last peaks in the spectrum, it is not possible to define a left midpoint or a right midpoint, respectively. Therefore, for these two peaks, the average distance between all of the peaks in the spectrum is used to define the left noise area and the right noise area. The left noise area of the first peak is defined by the position of the first peak minus half the average peak distance, while the right noise area of the last peak is defined by the position of the last peak plus half the average peak distance.

When only one peak is present in the spectrum, the noise is calculated by first finding the points to the left (and the right) where the (smoothed) first-order derivative is no longer positive (or negative). The noise at the peak is then the linear interpolation of these two values.

The OSNR tool analysis window is by default displayed in the region below the main data display area, but can be displayed in a floating window (see Section 3.8.1 Floating Windows).

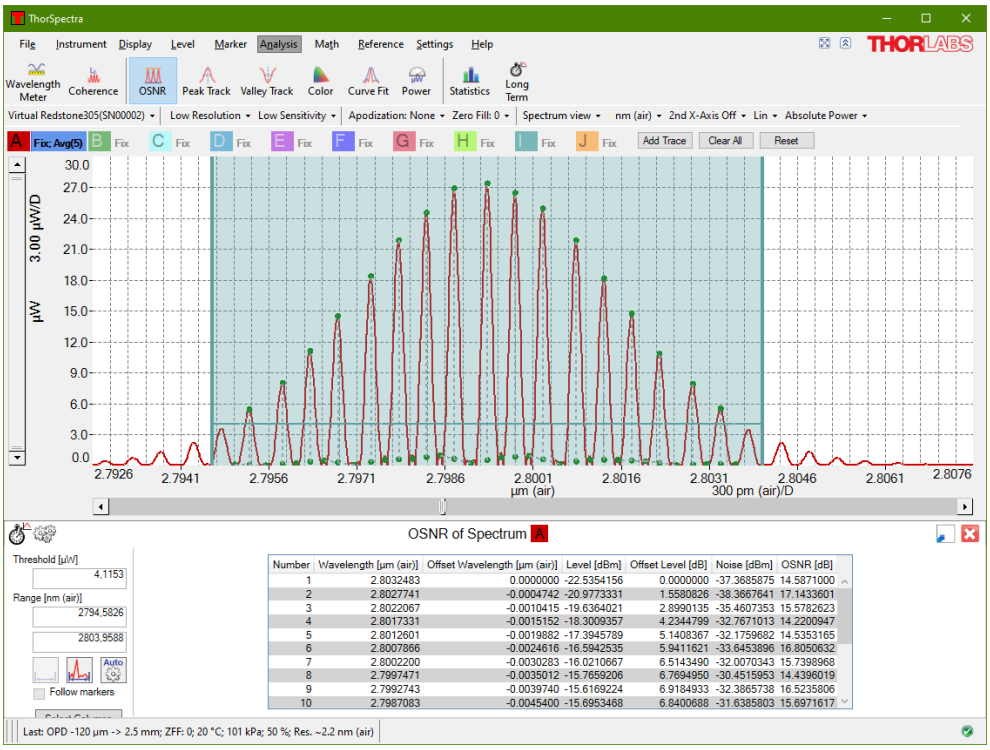


Figure 32. Optical Signal-to-Noise Ratio (OSNR) Analysis Tool

3.8.4. Peak Track

Through the Peak Track analysis tool it is possible to track the position, amplitude, and width of peaks in the spectrum over time. The maximum number of peaks that can be simultaneously tracked is 2048.

When the Peak Track tool is active, the peak track analysis window will by default be displayed below the main data display area (see Figure 33). Here, a data table shows information about the peaks, as well as a small toolbox with the settings that were used to find the peaks. It is also possible to select which columns are displayed in the data table by clicking on “Select Columns.”

The criteria used to find the peaks are:

- **Threshold**: Only data points with values higher than the threshold will be considered when searching for peaks.
- **Range**: Limits the x-axis range over which the search for peaks is performed.
- **Maximum Number of Peaks** (found in the Settings dialog box behind the cogwheels icon): Limits the number of peaks returned by the Peak Track analysis tool. The default value is 20 peaks; the maximum value is 2048 peaks.
- **Min Peak Height (dB)** (found in the Settings dialog box behind the cogwheels icon): Only peaks which have a peak-to-baseline ratio of at least this value will be returned.

When the Peak Track tool is active, the currently Active spectrum trace is checked for peaks upon the collection of a new spectrum from the instrument. By default, the peaks are sorted in order of decreasing intensity. Right-

clicking in the data table brings up a contextual menu from which it is possible to save the data in the data table to file or copy the data to the clipboard for analysis in another software.

The peaks found in Peak Track can be tracked over time in a Long-Term Analysis (see Section 3.8.10). Note that since the peaks are ordered by decreasing intensity, they will be rearranged if the relative intensity of the peaks in the spectrum changes.

If no peaks are found by the Peak Track tool, check the Threshold and Min Peak Height settings to make sure that the expected peaks in the spectrum are higher than these constraints. The settings can be changed either in the Settings dialog box (described in Section 4.2 Peak Track Settings) or directly in the tool options panel found to the left of the data table in the Peak Track analysis window.

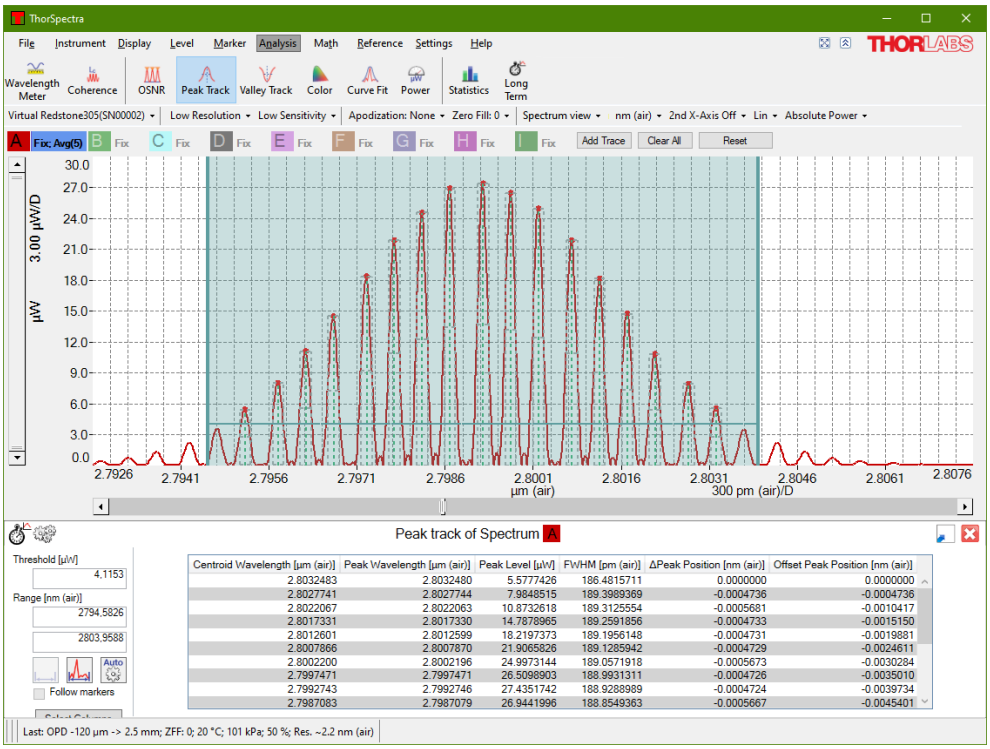


Figure 33. Peak Track Tool with Range and Threshold Lines (in Blue)

For each peak that is found in the currently Active Trace, one line is displayed in the table shown in the Peak Track analysis window (by default found below the main data display area). The data reported for each peak is as follows:

- **Centroid Location**: The x-axis location of the center of mass of the peak. This location is determined from the weighted average of all points whose intensities do not fall below the Min peak height level defined in the Peak Track analysis window.
- **Centroid Level**: The value of the trace at the center of mass of the peak, defined as explained above.
- **Peak Location**: The x-axis location of the maximum value of the peak.
- **Peak Level**: The maximum peak value.
- **Width:** The width of the peak at “Min Peak Height” dB below the maximum value.
- **FWHM:** The full width of the peak at half of its maximum value.
- **Left Half-Width:** The x-axis distance from the maximum peak value to half of the maximum peak value, starting at the Peak Location and going in the direction of decreasing x.

- **Right Half-Width:** The x-axis distance from the maximum peak value to half of the maximum peak value, starting at the Peak Location and going in the direction of increasing x.

- **Baseline:** The value at which the base of the peak is found.

- **ΔPosition (Centroid or Peak):** The x-axis distance between the current peak and the previous peak in the table.

- **Offset Position (Centroid or Peak):** The x-axis distance between the current peak and the first peak in the table.

- **ΔLevel (Centroid or Peak):** The difference in level (either centroid level or peak level) between the current peak and the previous peak in the table.

3.8.5. Valley Track

Through the Valley Track analysis tool it is possible to track the position, depth, and width of valleys in the spectrum over time. The maximum number of valleys that can be simultaneously tracked is 2048.

When the Valley Track tool is active, the Valley Track analysis window will by default be displayed below the main data display area (see Figure 34). Here, a data table shows information about the valleys, as well as a small toolbox with the settings that were used to find the valleys. It is also possible to select which columns are displayed in the data table by clicking on “Select Columns.”

The criteria used to find the valleys are:

- **Threshold**: Only valleys where the local baseline has an intensity above the threshold will be found by the search.

- **Range**: Limits the x-axis range over which the search for valleys is performed.

- **Maximum Number of Valleys** (found in the Settings dialog box behind the cogwheels icon): Limits the number of valleys returned by the valley track analysis. The default value is 20 valleys; the maximum value is 2048 valleys.

- **Min Valley Depth (dB)** (found in the Settings dialog box behind the cogwheels icon): Only valleys which have a depth of at least this value (defined by the local baseline) will be found.

When the Valley Track tool is active, the Active Trace is checked for valleys upon the collection of a new spectrum from the instrument. By default, the valleys are sorted in order of increasing x-axis location. Right-clicking in the data table brings up a contextual menu from which it is possible to save the data in the data table to file or copy the data to the clipboard for analysis in another software.

The valleys found by the Valley Track tool can be tracked over time in a Long-Term analysis (see Section 3.8.10).

If no valleys are found by the Valley Track tool, check the Threshold and Min valley depth settings to make sure that the expected valleys in the spectrum are deeper than these constraints. The settings can be changed directly in the tool options panel found to the left of the data table in the Valley Track analysis window.

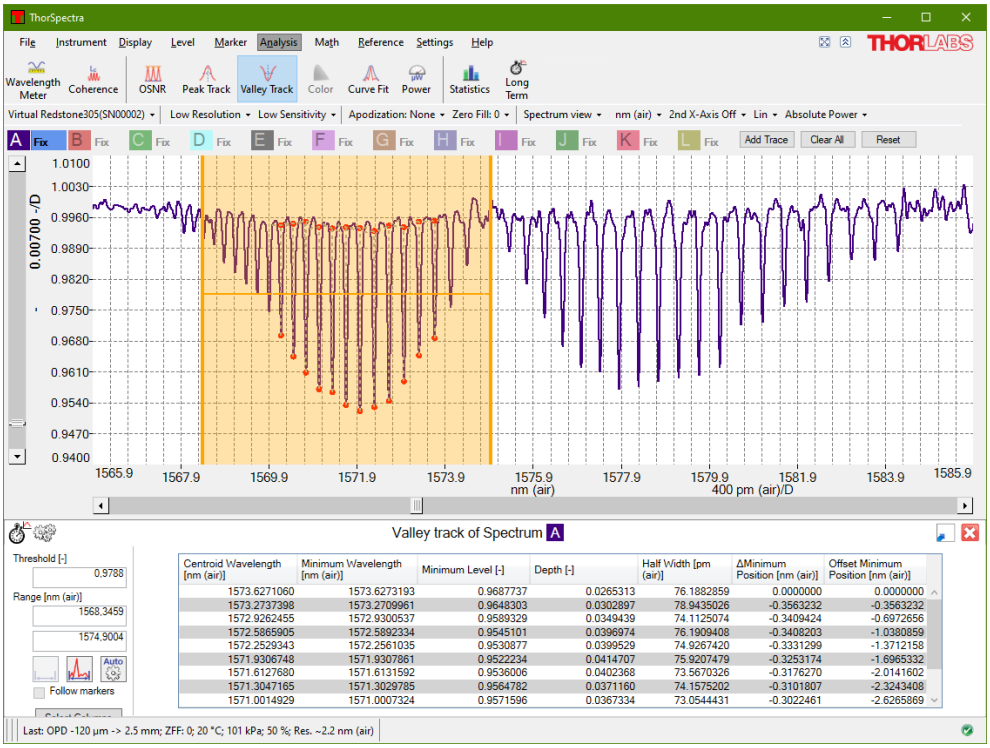


Figure 34. Valley Track Tool with Range and Threshold Lines (in Yellow)

3.8.6. Color Analysis

Color Analysis is only available for instruments covering the visible wavelength range [i.e., Item #s OSA201C, OSA202C, OSA302, CCT10, CCT11, CCT12, CCS100(/M), CCS175(/M), and CCS200(/M)]. For all other instruments, this tool will be disabled.

This tool analyzes the Active Trace. The CIE 1931, CIE 1960, or CIE 1976 color space can be chosen using the radio buttons below the graph. The software calculates the chromaticity coordinates and the main wavelength in the spectrum. CIE 1931 is the default color space.

The ThorSpectra software calculates the correlation between the collected spectrum and the three color matching functions x(λ), y(λ), and z(λ) defined from the CIE 1931 2° standard observer to obtain the tri-stimulus values X, Y, and Z. These are then normalized to obtain the chromaticity coordinates (x, y, and z) for the CIE 1931 color space, (u, v, and w) for the CIE 1960 color space, or (u', v', and w') for the CIE 1976 color space. The calculated chromaticity coordinates are displayed in the color space chromaticity diagram as a dark circle as well as displayed numerically next to the diagram.

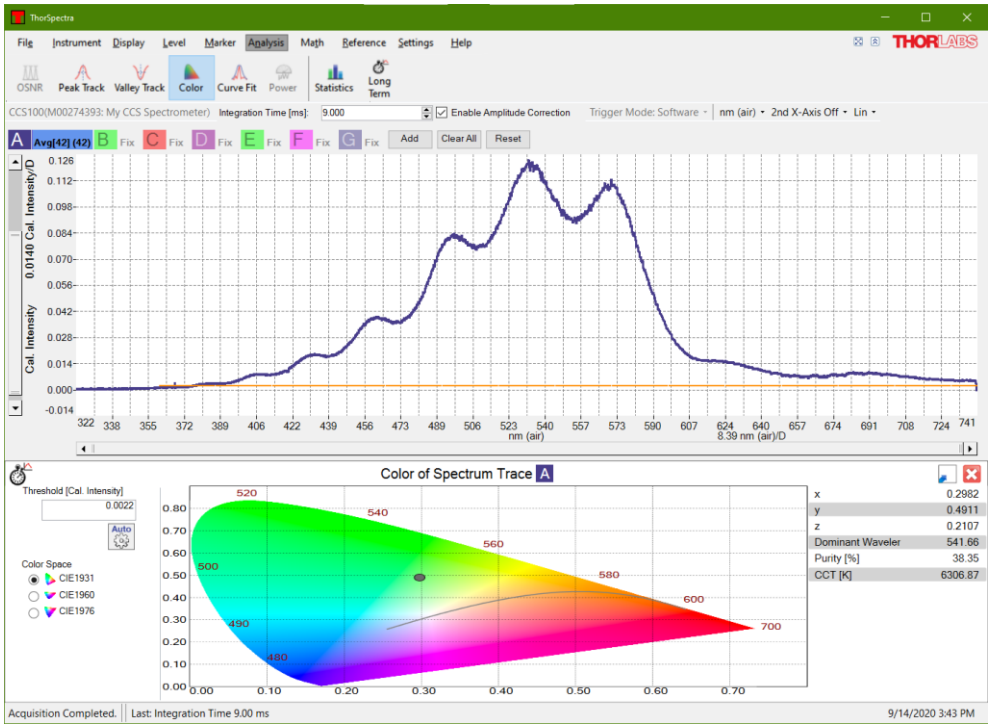


Figure 35. Color Analysis Tool. Calculated Chromaticity Coordinates as well as Main Wavelength displayed.

The main wavelength is calculated as the intercept between the straight line from the white point (1/3, 1/3) through the calculated chromaticity point (x, y) and the edge of the chromaticity diagram. The purity is calculated as the percentage of the distance from the white point (1/3, 1/3) to the edge of the chromaticity diagram that the distance from the white point (1/3, 1/3) to the calculated chromaticity point represents. A purity of 100% represents a point on the edge of the chromaticity diagram, i.e., a pure color, and a purity of 0% represents a mix of all colors, i.e., the white point itself.

The correlated color temperature can be calculated for a light source that is close enough to the Planckian locus in the 1960 UCS. The correlated color temperature is calculated by converting the calculated chromaticity point (x, y) into a point (u, v) in the CIE 1960 color space and finding the closest Planckian locus. If the distance to the closest Planckian locus ($\Delta_{u,v}$) is larger than 0.05, a temperature of -1 Kelvin is returned as an error code.

The threshold option (described in Section 3.8.2) makes it possible to ignore data points in the spectrum with low intensity; this can be useful if the spectrum is very noisy.

The Color Analysis window is by default displayed in the region below the data plot, but can be moved to a floating window (see Section 3.8.1 Floating Windows).

3.8.7. Curve Fit

The Curve Fit tool allows a mathematical function to be fit to an active trace over user-specified x-axis and y-axis intervals.

When the Curve Fit tool is enabled, an analysis window is docked below the main data display area. This window contains three parts. The leftmost section lets the user see and edit the x-axis range over which the mathematical curve is fitted, the middle section displays information about the fit, and the rightmost section displays the values of the fit parameters. The mathematical function used in the curve fit is a sum of different components. The following components can be used as terms in this function:

- Polynomials with an order from 0 to 9
- Gaussian

$$Ae^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- Lorentzian

$$\frac{A}{\left(\frac{x - x_0}{\frac{1}{2}w}\right)^2 + 1}$$

Please note that curve fitting is a computationally heavy process. If the data set is very large, the software might become unresponsive for a long period of time.

Defining the Function to Fit to the Trace

The fitting function is defined using the “Function Builder” dialog box (see Figure 36), which can be opened by clicking on the “Edit Function” button in the Curve Fit tool window (see Figure 37).

This dialog box is composed of three parts. The top contains two buttons that adds, modifies, or deletes function terms, the middle section displays the function used to fit the trace (labeled as the “Final Function”), and the bottom part displays the parameters of the currently selected function term. The currently selected term is outlined in black.

To add a new term to the Final Function, click on the “Add” button at the top of the dialog box, and a list of the available components will appear. To remove a term from the Final Function, click on the term, then click on the “Delete” button at the top of the dialog box.

By default, all parameters in each term of the Final Function are scaled in order to best fit the analyzed trace. To reduce computational time, parameters can be set to fixed values, thereby preventing them from being scaled. To do this, select the term, check the “Fixed” check box for the parameter you wish to fix, and type the desired fixed value into the “Value” column.

Please note that it is not possible to fit multiple polynomials simultaneously; the Final Function may only contain one polynomial term (which may have order up to 9).

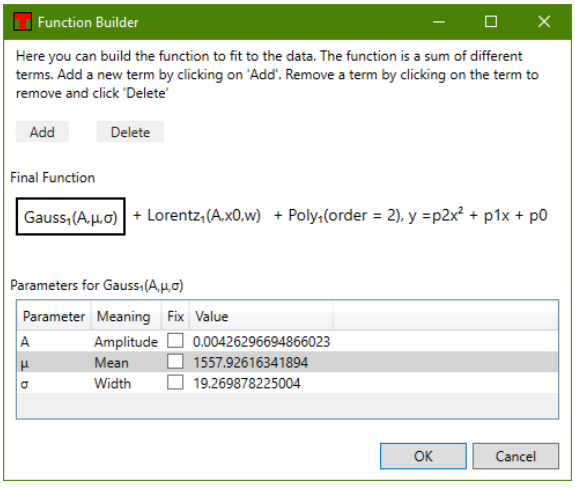


Figure 36. The fitting function is defined using the Function Builder dialog box.

Getting the Result

When the fit is finished, the fit parameters as well as the values and standard errors thereof are displayed in a table in the Curve fit tool window. The fitted curve is also overlaid on the data in the main data display area for visual inspection.

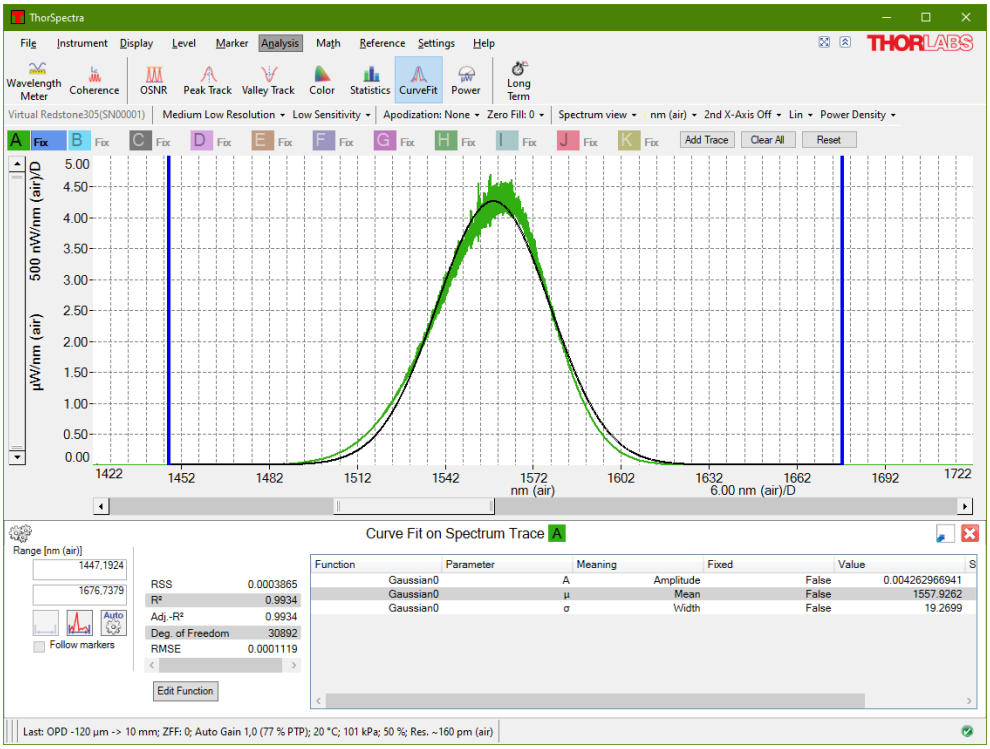


Figure 37. Curve Fit Tool

The middle table shows the properties of the fit itself. The following parameters are displayed:

- **RSS (residual sum of squares):** This is the sum of the squared differences between the fitted function and the trace, taken over all data points included in the fit.
- **R^2:** This is calculated as:

$$R^2 = 1 - \frac{RSS}{TSS}$$

  where $\boldsymbol{RSS}$ is the residual sum of squares, and TSS is the total sum of squares, calculated as the sum of the squared differences between the trace and the average value of the trace, taken over all data points included in the fit.

- **Adjusted R^2:** This is the **R^2 value** above adjusted for the degrees of freedom. This is calculated as:

$$\text{Adjusted } R^2 = 1 - \frac{RSS(n-1)}{TSS(n-p-1)}$$

  where n is the length of the data set in the fitted region and p is the number of fitted parameters.

- **Degrees of Freedom:** This is the length of the fitted data set minus the number of fitted parameters.
- **RMSE (root mean square error):** Calculated as the square root of the RSS divided by the **Degrees of Freedom**.

3.8.8. Power Analysis

Power Analysis tracks the incident optical power into the spectrometer. The optical power is calculated by integrating the Active Trace over an x-axis range.

The Power Analysis tool is displayed in a floating window by default, but can be docked below the main display area, as described in Section 3.8.1. It displays the optical power, integrated over some wavelength or frequency range, in the current y-axis units (mW or dBm). The x-axis range over which the power is integrated can be

modified either by dragging the range lines or by typing new values into the input boxes (described in Section 3.8.2). Changes to the range will take effect immediately.

Movable markers 1 and 2 (see Section 3.4) can also be used to specify the analysis range. Enabling the markers activates the “Get From Markers” button located below the two input boxes. Pressing this button retrieves the positions of the two movable markers and recalculates the optical input power. The interval can also be defined by the range of the currently displayed data by pressing the “Use Displayed Range” button found below the input boxes.

Note that zooming or scrolling the graph will not automatically change the interval.

The Power Analysis window shows the minimum, maximum, mean, and standard deviation of the optical powers that have been measured while the Power Analysis tool has been active. The values are updated after every new sweep and are reset if the x-axis range is changed. The statistics can also be reset by clicking the “Clear” button.

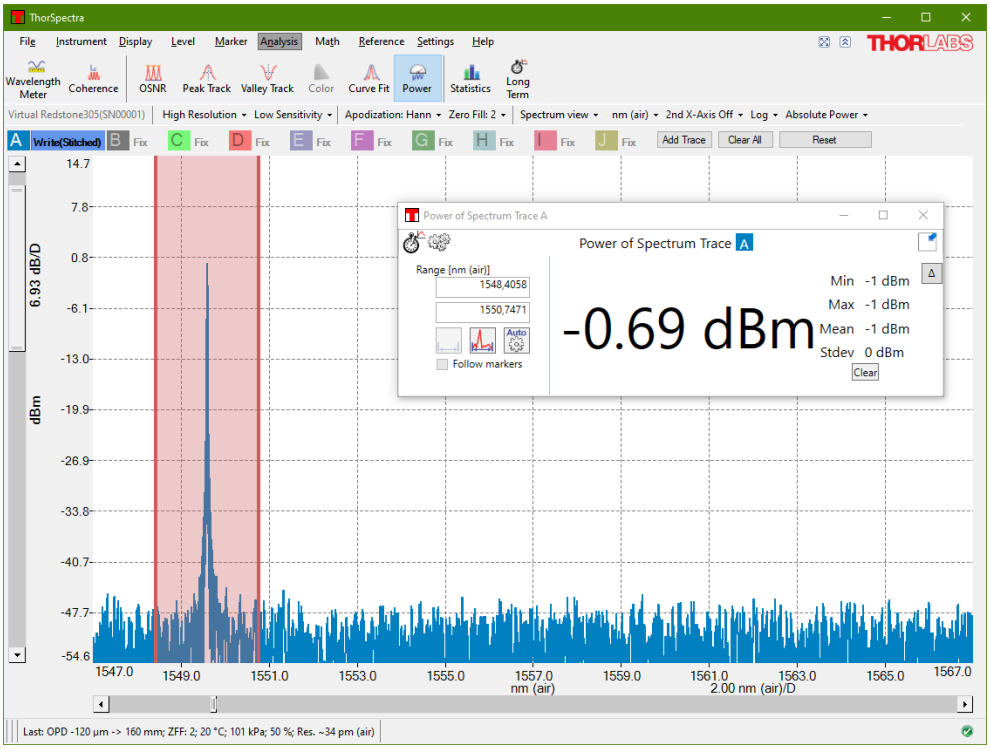


Figure 38. Power Analysis Tool

If Dark Room mode (Section 3.2.11) is activated while the Power Analysis tool is active, the display will not be “dark” until the window is closed and reopened.

3.8.9. Statistics Analysis

Statistics Analysis allows several statistical parameters of a trace to be analyzed and tracked over time over a user-specified x-axis interval. It is possible to statistically analyze raw data (i.e., live spectra), calculated values (i.e., transmittance or absorbance), and arbitrary user-defined traces (e.g., traces composed from algebraic manipulations of other traces).

When the Statistics Analysis is enabled, the statistics analysis window is displayed in a floating window or docked below the main display area, as described in Section 3.8.1. This window contains a data table with statistical information about the Active Trace over the x-axis range defined by the values in the boxes in the tool options panel. Either end of this range can be changed either by typing new values into the boxes or by dragging the range lines in the main data display area (described in Section 3.8.2). Changes will take effect immediately.

Movable markers 1 and 2 (see Section 3.4) can also be used to specify the analysis area. When these markers are enabled, a “Get From Markers” button located under the two input boxes is activated. Clicking this button

defines the endpoints of the analyzed interval as the locations of the two movable markers and recalculates the result.

Finally, the interval can also be defined by the current displayed range of the main data display range by clicking the “Use Displayed Range” button below the input boxes. Note that the input boxes are only visible if the window is large enough.

Note that zooming or scrolling the graph will not automatically change the interval.

The following statistical parameters are available:

- **Mean:** The mean (average) value of the trace over the analyzed interval.
- **Variance:** The sample (i.e., not the population) variance of the trace over the analyzed interval. This is calculated using the following formula:

$$\frac{1}{N-1}\sum_{i=1}^{N}(x_i-\bar{x})^2$$

  where N is the number of samples and $\bar{x}$ is the average value over the analyzed range.
- **Standard Deviation:** The sample standard deviation of the trace over the analyzed range. This is the square root of the sample variance above.
- **RMS:** The root mean square (RMS) value of the trace over the analyzed range.
- **Weighted Average:** The average x-axis value over the analyzed range, weighted by the absolute value of the y-axis.
- **Minimum Value:** The smallest value of the trace over the analyzed range.
- **Maximum Value:** The largest value of the trace over the analyzed range.
- **Number of Values:** The total number of values in the over the analyzed range.
- **Contains NaN:** Equal to true if the trace contains a data point with a “Not a number” value in the analyzed range, and equal to false otherwise.
- **Contains Inf:** Equal to true if the trace contains a (positive or negative) infinite value in the analyzed range, and equal to false otherwise.

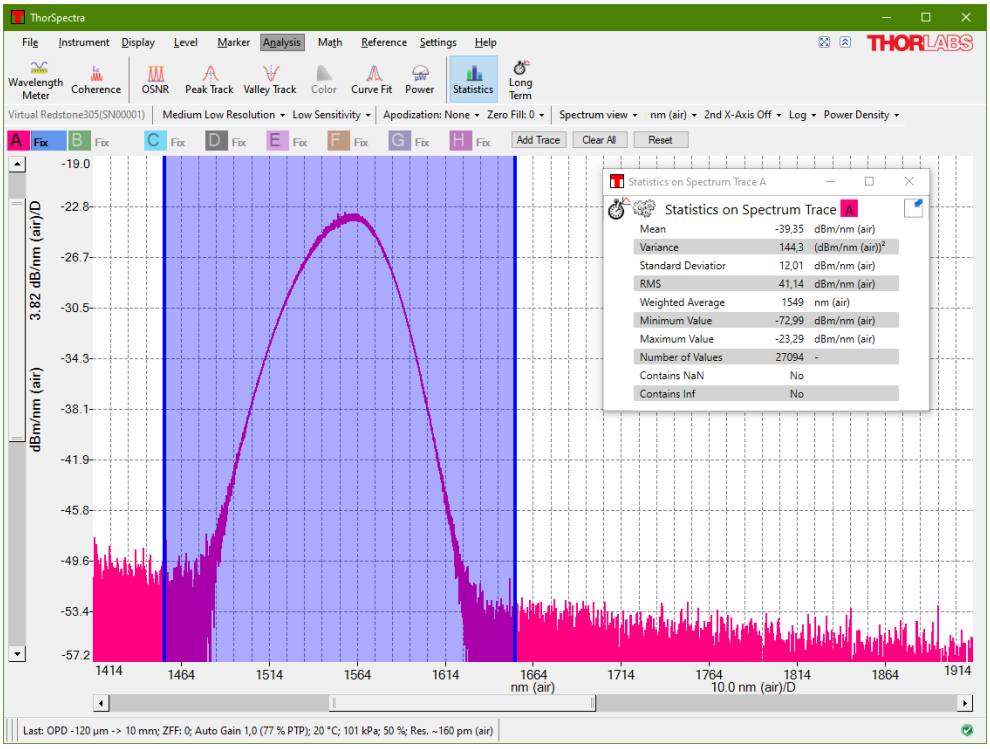


Figure 39. Statistics Analysis Window

3.8.10. Long-Term Analysis

The Long-Term analysis tool is intended for long-term monitoring of optical systems. These tests can track any output parameter from the analysis tools as well as status parameters of the connected spectrometers.

Setting Up and Running

A long-term test can be started in two ways: by clicking on the “Long-Term” button available in the upper left corner of each analysis tool window, as shown in Figure 40, or by clicking the “Long-Term” button under the Analysis menu. When starting a long-term test directly from an analysis window, only the parameters from the active analysis tool can be tracked. In contrast, the button found under the Analysis menu enables tracking of all parameters available for long-term tracking.

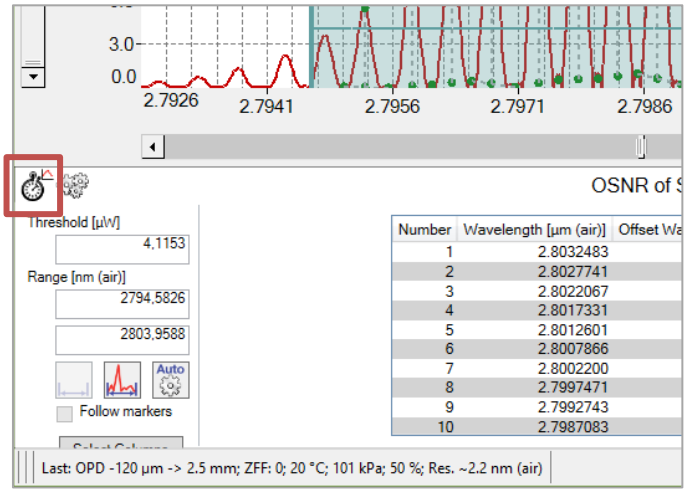


Figure 40. Location of the Long-Term Analysis Button in an Analysis Tool Window

Clicking on Analysis and “Long-Term” will open a dialog box where the parameters to be monitored can be selected, as well as the desired duration of the test.

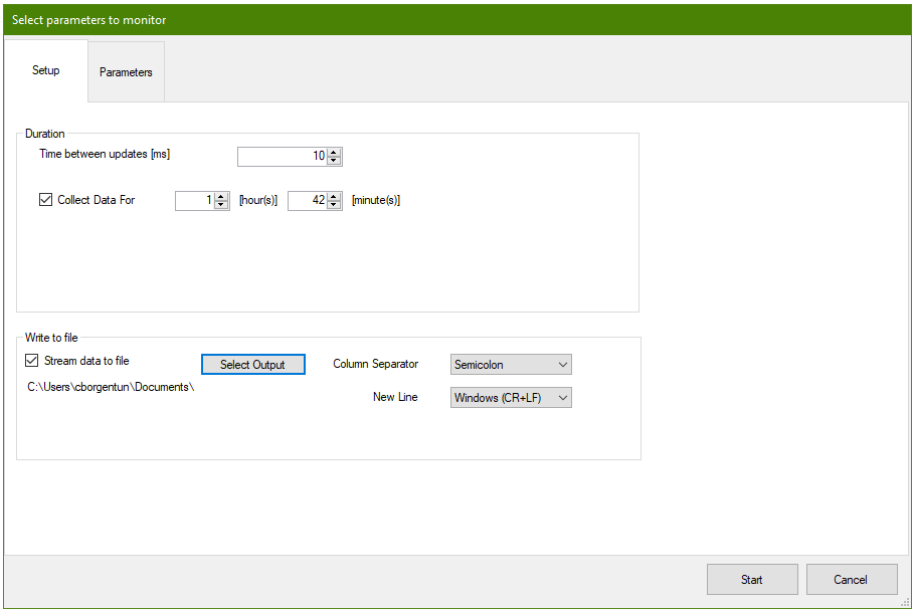


Figure 41. Setting Up the Long-Term Analysis – General Setup

The general options can be selected from the “Setup” tab in this dialog box, see Figure 41. The duration of the test can be specified in hours and minutes. If the duration is set to zero, the measurement will run until the “Stop” button is pressed. The time interval between each two updates can be set by selecting/writing a value in the box “Time between updates.” Note that this only defines the minimum time between the updates of the measurement; the actual rate will be determined by the update rate of the instrument.

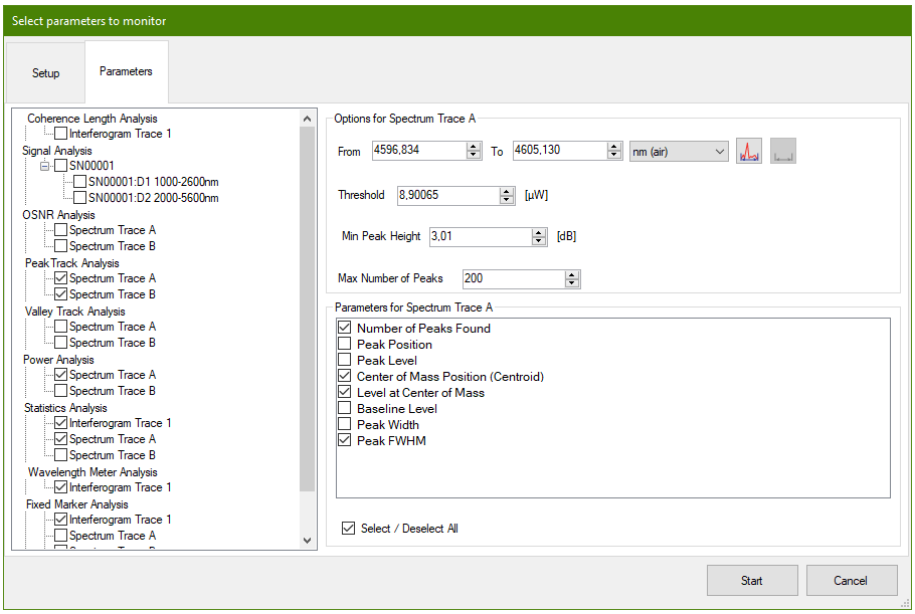


Figure 42. Setting up the Long-Term Analysis – Selecting Parameters to Track

The parameters to track can be selected in the “Parameters” tab of the Long-Term setup dialog box. The left section of the dialog shows the types of parameters which can be collected. Selecting one group shows the available parameters and the options for the collection in the right section. For example, selecting “Peak Track Analysis” will show controls where the x-axis range in which to track peaks, the threshold, the minimum peak height, and the maximum number of peaks can be defined (see Figure 42).

Note: To track a parameter, both the parameters group (e.g., “Peak Track Analysis”) **and** the parameter to track (e.g., “Peak Position”) **must** be checked.

When the settings have been completed in the Long-Term setup dialog box, press the “Start” button found in the lower right corner. This will open the Long-Term window, showing one graph for each parameter being collected as well as a menu with options for managing the Long-Term analysis.

When opening the Long-Term setup via a specific analysis tool window, the setup window is simpler because only the parameters of the current analysis tool will be available for setup (see Figure 43). In the setup window the trace from which the data will be collected can be selected, whether or not to stream the data to a file as well as options and parameters to track. Note that it is not possible to set the duration of the Long-Term analysis in this setup; the measurement will continue until the “Stop” button is pressed.

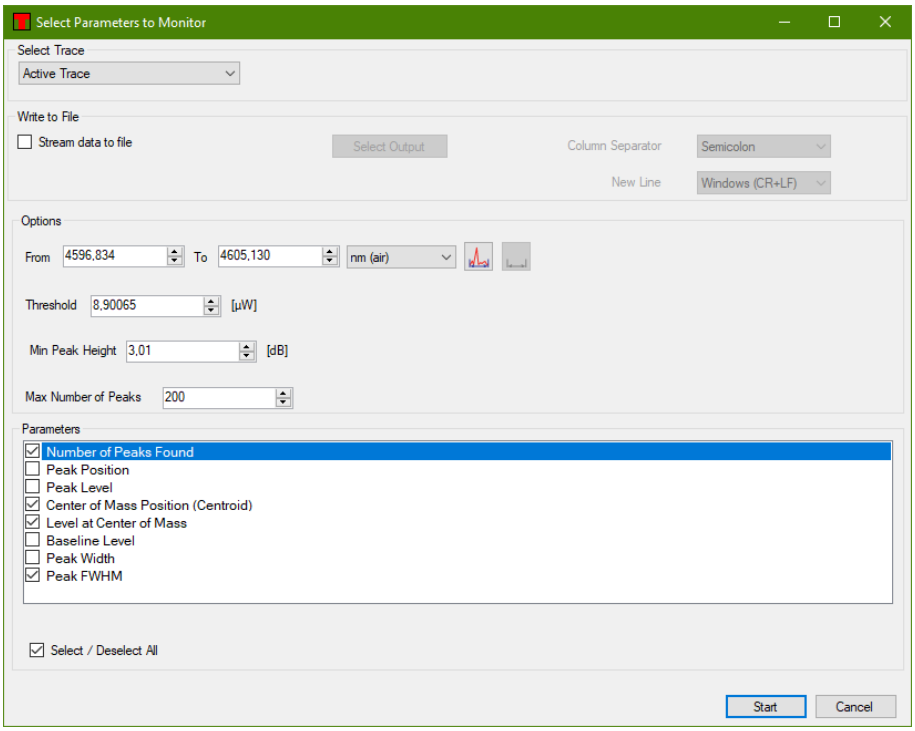


Figure 43. Setting Up the Long-Term Analysis – Opened From an Analysis Tool Window

Storing Results

The data collected by the Long-Term tool can either be streamed to disk, meaning that the data will be written to a file as soon as it is collected, or it can be stored to file after the collection has been done.

To stream the collected data to disk, check the button “Stream data to file” found in the “Setup” tab of the Long-Term setup dialog box (see Figure 41) and select a directory in which to store the data. Streaming data to file will create one file per parameter group (e.g., Peak Track data or device status data) and will write one line in this file for every spectrum that is collected from the instrument.

When the Long-Term collection has been stopped (see below) it is possible to store the collected data to file. This is done by pressing the “Save” button in the Long-Term window. This will store all the collected data into one file.

Stopping and Restarting

To stop a Long-Term measurement that has been started, press the “Stop” button in the Long-Term window which was opened when the test started (note that this window may be hidden behind the main window of the ThorSpectra software).

Each graph in the window can be minimized by clicking on the small icon to the left of the parameter name. This will automatically make the other graphs in the dialog larger.

The topmost part of the window displays the status of the measurement. The current duration of the test will be displayed and if a time limit is set on the test, this will also be displayed. If data is streamed to file, this will display a button opening the location of the files.

When the “Stop” button is pressed it will transform into a “Continue” button. Pressing this will continue the Long-Term measurement where it was left off and will use the same parameters.

To clear the Long-Term measurement of collected data, stop the measurement and press the “Clear Data” button. The measurement can then be restarted by clicking on “Continue.”

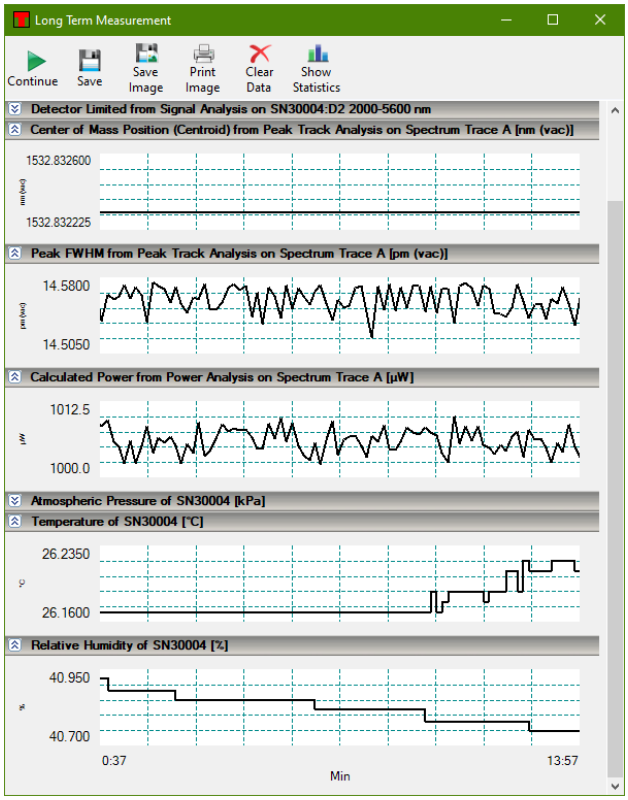


Figure 44. Long-Term Window

The results of the measurement can be stored to file by pressing the “Save” button and a screenshot of the measurement can be stored as an image file or printed by pressing the “Save Image” or “Print Image” buttons.

3.9. References

3.9.1. Reference Databases (e.g., HITRAN)

ThorSpectra ships with built-in spectroscopic reference standards from the HITRAN database (**https://hitran.org**) for acetylene (C_2H_2), water vapor (H_2O), and carbon dioxide (CO_2). These standards can be used to identify these gases in acquired spectra. To identify other foreign constituents of an acquired spectrum, the ThorSpectra software can import additional HITRAN reference standards, as well as reference spectra saved in any of the other export formats that the software supports (see Section 3.7 Saving and Loading Data). This allows the user to acquire, analyze, and save a baseline spectrum that is specific to a given lab environment.

Saved spectra are used directly by ThorSpectra without further modification. On the other hand, HITRAN standards (sometimes referred to as ”line-by-line references”) must be converted to a spectrum before they can be used in further analysis. This conversion is detailed below.

Importing References

The Reference database window displays the currently available references. This window is opened by clicking on the “References” button in the Reference menu in the main window. To add a new reference, open this

window and click the “Import” button. HITRAN line-by-line references must have the .par file extension and be saved in HITRAN’s 160-character format.

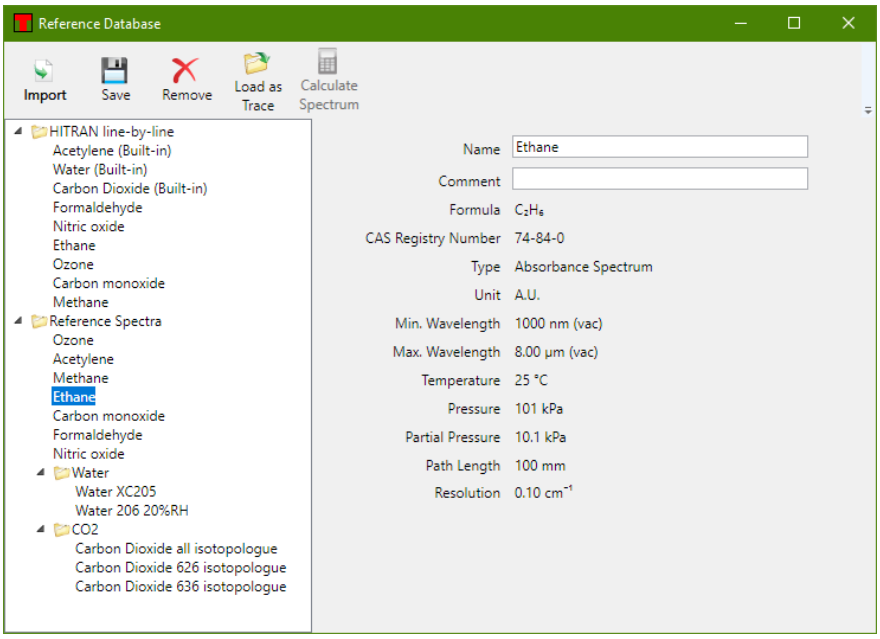


Figure 45. Reference Database Window

Converting HITRAN References into Absorption Cross Sections, Absorption Spectra, or Transmission Spectra

A line-by-line reference must be converted into a regular spectrum before it can be used in the software. This spectrum will be used during the Reference fitting step to help account for line-shifts, modulations in line intensity, line broadening caused by air, and self-broadening. To obtain a regular spectrum, an *absorption cross section* must first be calculated.

An absorption cross section is a physical property of a molecule that describes how strongly the molecule absorbs light at a particular wavelength. It is denoted by $\sigma(\lambda)$ in the Beer-Lambert law:

$$I(\lambda) = I_0(\lambda)\, e^{-\sigma(\lambda)\cdot cL}$$

Here, I is the light intensity after absorption, I_0 the incident light intensity, λ is the wavelength, $\sigma(\lambda)$ is the wavelength-dependent absorption cross section, c is the concentration of the gas of interest, and L is the total path length traversed by the light as it passes through the gas. The calculated absorption cross section has units of *cm²/molecule*.

The absorption cross section is related to the *absorption coefficient*, denoted by k. The absorption coefficient can be calculated by multiplying the absorption cross section by the so-called *mass path*

$$k(\lambda) = \frac{qP}{k_B T}\sigma(\lambda)$$

where q is the volume mixing ratio of the gas, P is the total pressure, k_B is Boltzmann’s constant, and T is the temperature.

The ThorSpectra software considers the total pressure, the partial pressure of the gas of interest, and the temperature in order to calculate the absorption cross section and resulting spectrum. By clicking the “Calculate Spectrum” button, the following dialog box will appear, which displays all the needed input parameters. Please note that the usable x-axis data range will be limited by the data range from the HITRAN line-by-line reference.

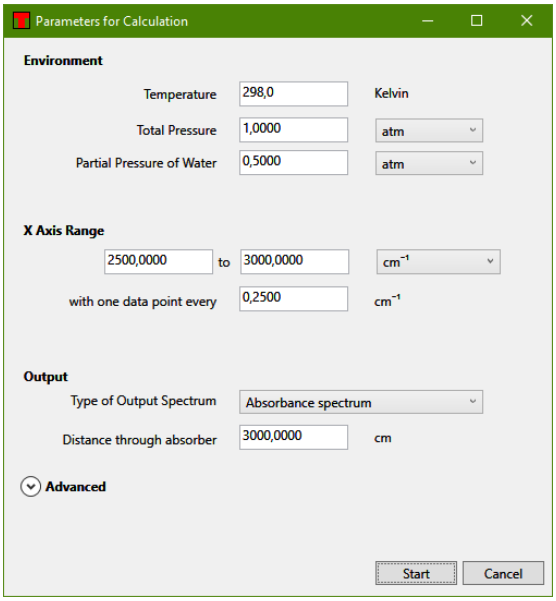


Figure 46. Reference Spectrum Calculation Setup Window

This dialog box contains a drop-down menu that allows the user to choose the absorption cross section, absorption spectrum, or transmission spectrum as the output of the calculation. Please note that if an absorption or transmission spectrum is desired, the dialog box will prompt the user to enter the optical path length through the gas of interest; the absorption cross section is independent of the path length.

Loading Traces

Except for line-by-line references which have not yet been converted by the procedure outlined above, reference spectra can be loaded into the main ThorSpectra window and handled as any other trace. Simply click on the reference you wish to load in the Reference database dialog box and click “Load as Trace.” This will copy the reference to an empty trace in the main window.

3.9.2. Reference Fitting

The Reference Fit dialog box is used to assign peaks in an unknown spectrum to peaks from one or more reference spectra. To open this dialog box, click the “Fit” button in the Reference menu.

When the dialog box initially opens, the References section is displayed, which allows one or more reference spectra to be included in a fit by checking the “Include” check box. Fits can only be performed on measured absorbance or transmittance spectra, and references must be in the reference database (see Section 3.9.1) in order to be selectable.

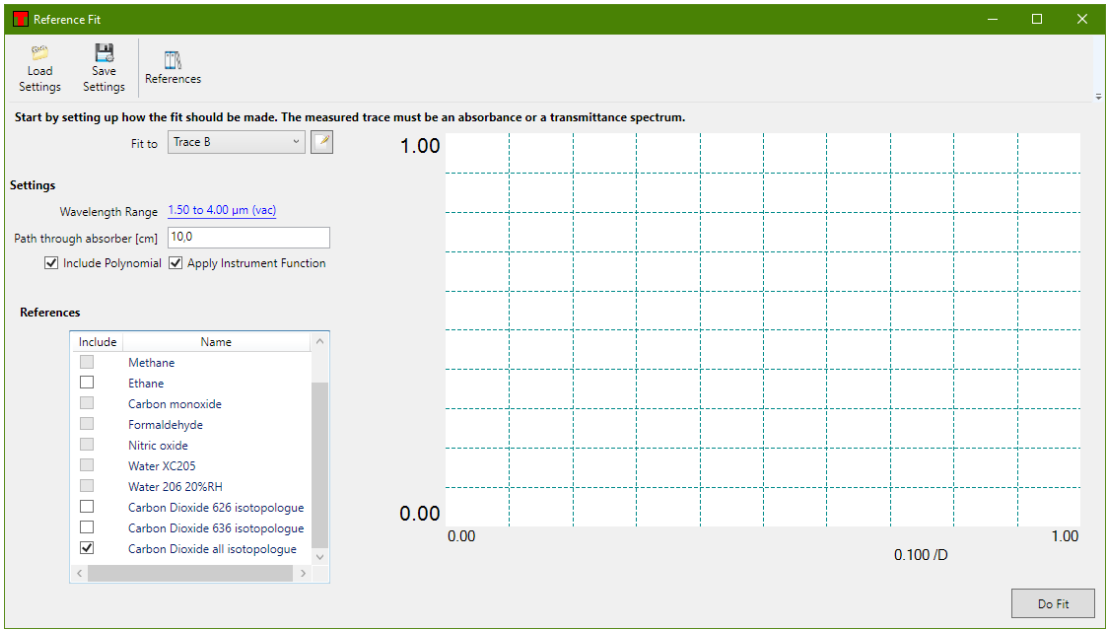


Figure 47. Setting Up a Fit in the Reference Fit Window

The wavelength range over which the fit is performed can be changed by clicking on the blue, underlined wavelength range in the Settings section. To perform the fit, click the “Do Fit” button. The Reference Fit dialog box will then contain a graph that displays the measured spectrum, each scaled reference spectrum, and the sum of all the reference spectra. To the left of the graph is a table that displays the fit coefficient for each reference spectrum that was used.

To try a different setup, click the “Back to Setup” button.

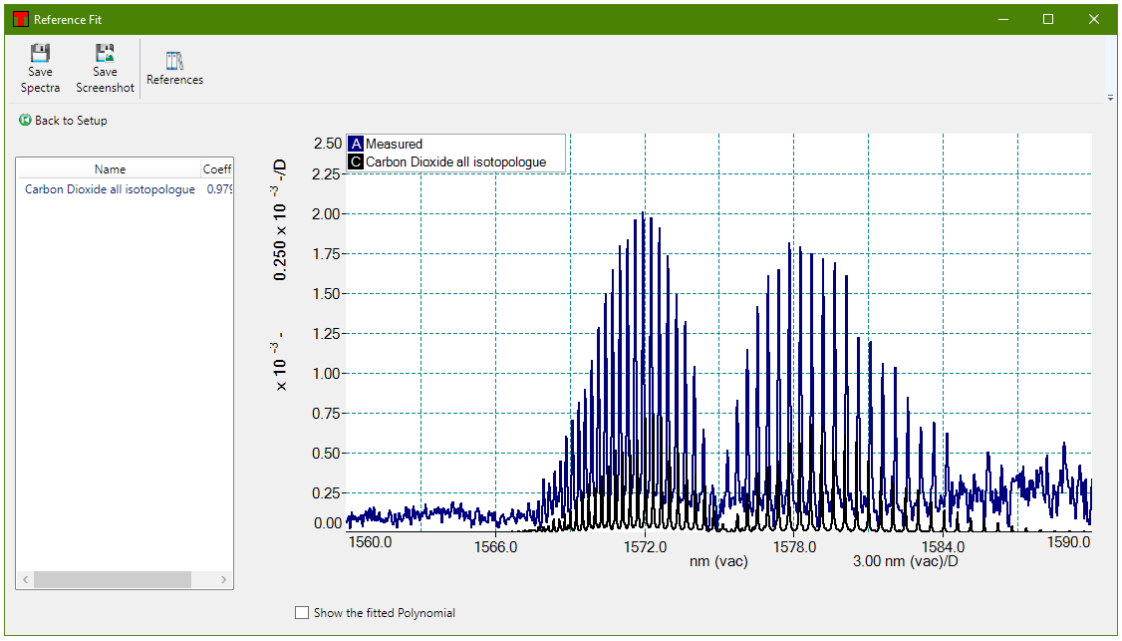


Figure 48. The Result of the Fit Displayed in the Reference Fit Window

3.9.3. Baseline Correction

The Baseline Correction operation is only available for spectrum traces. As shown in Figure 49, the Baseline Correction function removes baseline absorption from an acquired spectrum.

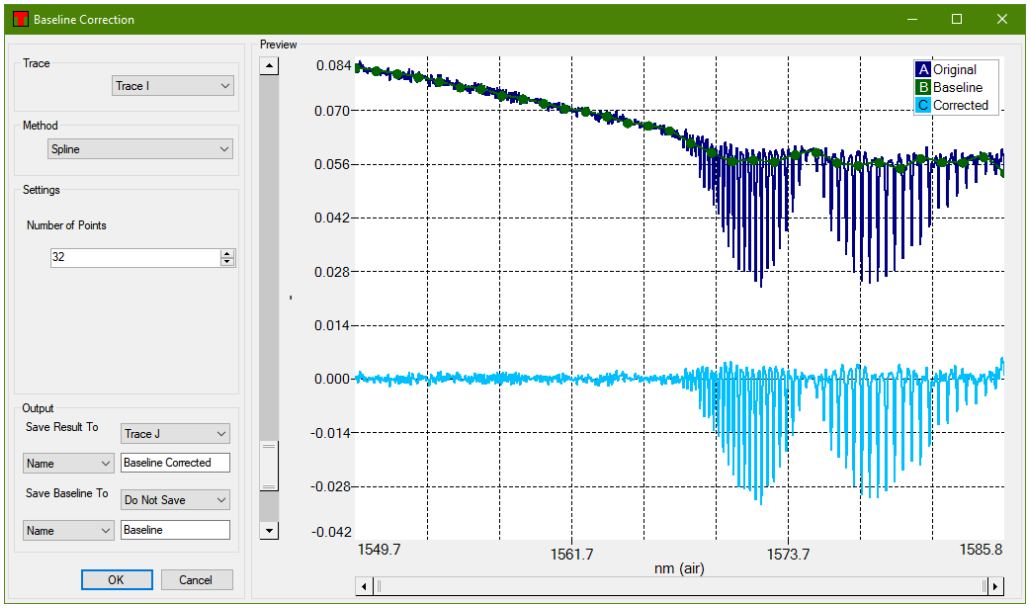


Figure 49. Baseline Correction Window

To perform a baseline correction, click the “Baseline” button in the Reference menu. The Baseline correction dialog box, which allows you to adjust the baseline correction while viewing the results of your adjustments in real time, will appear.

Baseline correction can only be performed on one trace at a time. Select the trace you wish to correct from the Trace drop-down menu in the upper left corner, then select the correction method from the Method drop-down menu directly below. There are four available methods:

- **Spline**: *N* baseline points linearly spaced are placed along the trace, and the local median value is determined around each point. The baseline is then calculated as a cubic Hermite spline, fitted to the locations and local median values of the *N* baseline points. The baseline points are displayed in the graph in the dialog box, and can be dragged around freely to adjust the baseline. The number of points to base the calculation upon can be set by the Settings drop-down menu below the Method drop-down menu.

- **Polynomial**: The baseline is determined by fitting a polynomial to the entire trace. The Settings drop-down menu allows the order of the polynomial to be set.

- **Polynomial Below**: The baseline is determined by fitting a polynomial to a set of baseline points. These points are chosen iteratively. In the first iteration, the entire trace is fit to the polynomial. Next, the points in the trace that lie below the fitted polynomial are used to designate a new set of baseline points. These steps are repeated until either no more points can be excluded, or the number of baseline points is less than (*polynomial order* + *1*).

- **Polynomial Above**: The baseline is determined in the same fashion as the **Polynomial Below** method, but points lying above the fitted polynomial are selected instead.

The input trace, the calculated baseline, and the final corrected trace will be displayed in the Baseline Correction dialog box. When you are satisfied, use the Output drop-down menu to select the trace to which you wish to export the corrected trace, and click “Ok.” The corrected trace will appear in the main window.

3.10. Keyboard Shortcuts

- **Ctrl+N**: Collect a new single spectrum

- **Ctrl+R**: Start/stop repeated measurements

- **Ctrl+I**: Show information about the currently Active Trace
- **Ctrl+L**: Toggle between linear and logarithmic scaling
- **Ctrl+1**: Enable/disable movable line marker #1
- **Ctrl+2**: Enable/disable movable line marker #2
- **Ctrl+3**: Enable/disable movable level marker #3
- **Ctrl+4**: Enable/disable movable level marker #4
- **Ctrl+O**: Load one or more traces from a file
- **Ctrl+S**: Save a trace to a file
- **Ctrl+Shift+S**: Save all traces to a file
- **Ctrl+Alt+S**: Save all visible traces to a file
- **Ctrl+P**: Print a screenshot of the currently displayed window
- **Ctrl+Z**: Undo the last math operation performed (if any)
- **Ctrl+Y**: Redo the last math operation undone (if any)
- **Ctrl+"+"**: Zoom into the graph
- **Ctrl+"-"**: Zoom out from the graph
- **Ctrl+Left Arrow**: Move the graph one step to the left
- **Ctrl+Right Arrow**: Move the graph one step to the right
- **Ctrl+PageDown**: Set the Active Trace to the trace after the one that is currently active
- **Ctrl+PageUp**: Set the Active Trace to the trace before the one that is currently active
- **Alt+W**: For the currently Active Trace, toggle status between "Write" and "Fixed"
- **Alt+F**: Set the Active Trace to "Fixed"
- **Alt+A**: Opens the Average options dialog when it is possible to set the Active Trace to "Average"
- **Delete**: Clear the currently Active Trace

Chapter 4 Settings

Pressing the Settings button in the main menu will open the Settings dialog. When a device is connected, an Active Device page will appear which is specific to the connected device. Please refer to the instrument manual for information regarding that page. Below are described the pages common to all instruments.

4.1. Display Settings

On the Display page it is possible to change the properties of the display, such as the background color of the display and the number of traces used. Note that the color of each trace is not changed here; instead see Section 3.6 Working with Data in Traces.

The Line Width option changes the width of the lines used for drawing the traces in the main data display. Using thicker lines can be beneficial if the screen is located at a distance from the operator or the screen is hard to read.

The legend drop-down menu enables or disables the legend of the main data display area and makes it possible to select what text data to display in the legend, see Section 3.2.10 Displaying a Legend in the Data Display Area.

If the check box “Show Individual Data Points” is checked, the display will show crosses at the individual data points in the traces when the graph is zoomed in so much that only one hundred data points are drawn.

The check box labeled “Interferogram in Percent” (only available for interferogram instruments in Advanced level) toggles between showing the interferogram as percent of the full measurable range (default) or in “counts” on the ADC. See also the Section 3.2.5 Setting the Unit of the Vertical Axis.

If the check box “Activate Persistence” is checked, the display will also display the last few spectra acquired in a more faded nuance.

***Note*:** Enabling persistence might severely slow down the update rate of the screen.

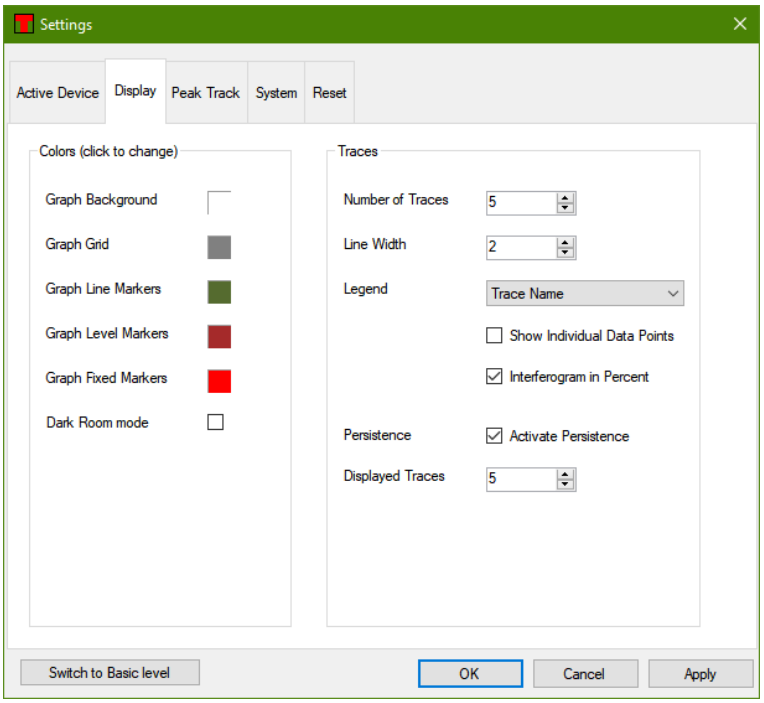


Figure 50. Display Settings Page

4.2. Peak Track Settings

The automatic Peak Track routine uses a number of parameters for finding peaks in the spectra. These options are the same as can be specified in the options panel for the Peak Track analysis tool (see Section 3.8.4 Peak Track).

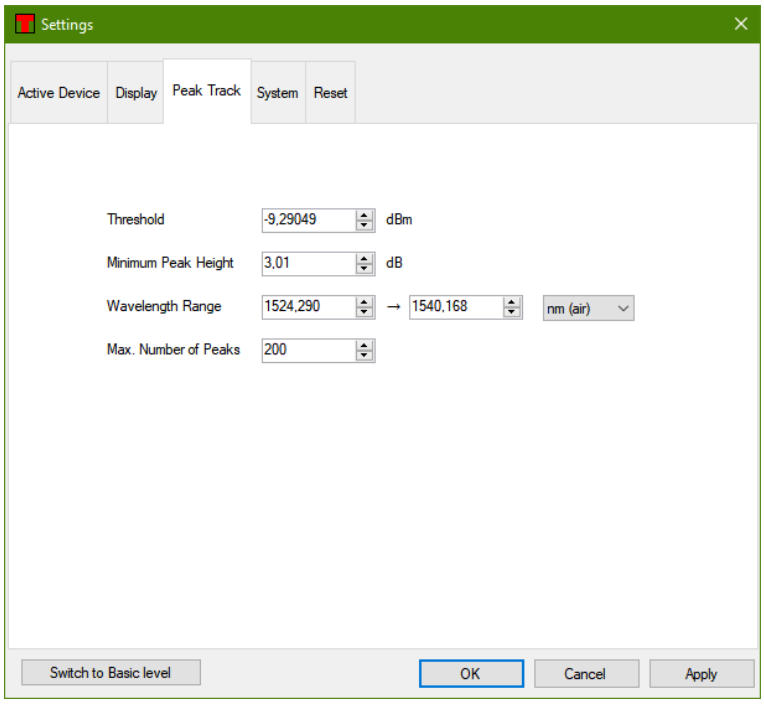


Figure 51. Peak Track Settings Page

- **Threshold**: Only peaks with a peak intensity higher than this given threshold level will be returned by the automatic peak track algorithm. Use this to reject noise peaks in the spectrum.

- **Minimum Peak Height (dB)**: The automatic peak track algorithm will only return peaks with a peak-to-baseline ratio higher than this value. Use this parameter to reject low peaks in the spectra. Note that this value is in dB (i.e., a Min peak height of 3.0 dB corresponds to the peak level being a factor of two higher than the local baseline).

- **Wavelength Range (or Frequency Range)**: The automatic peak track algorithm will only return peaks located between the two given wavelengths (or frequencies). Please note that the label and units of this setting will depend upon the x-axis units selected by the user. For instance, the label will read "Frequency Range" and the units will be THz, if THz is selected as the x-axis unit.

- **Max Number of Peaks**: The automatic peak track algorithm will only return as many peaks as specified here. The maximum value is 2048, and the default value is 20. Please note that higher values here can degrade the performance of the software, since lower-intensity peaks are more difficult to find.

4.3. System Settings

The name of the instrument operator can be entered here, which will be stored in the trace header.

The drop-down menu "Power Down Devices After" (not available for all instruments) allows the user to select the duration of inactivity after which the connected devices will power down to conserve energy. By checking the check box "Ignore Interferogram Traces' Status", the devices can power down even if the status of an interferogram trace is set to collect data, i.e., "Write" or "Average" etc.

By default, the display will clear data from traces with "Write" status when any device acquisition settings are changed. By unchecking the check box "Clear data when Acquisition Settings Change," this behavior is changed to only clear data from a trace when new data has been collected or either the "Clear All" button or a clear option has been selected from the Trace menu.

4.4. Reset

To completely reset all settings to their original default values, press the button “Restore Settings to Default” found under the “Reset” page. Note that this action cannot be undone.

4.5. Saving and Loading Settings

When the ThorSpectra software closes, it will store the currently used settings to file and restore them during the next startup. However, when alternating between different sets of settings it can be beneficial to store settings to file and restore these at a later time.

To store the currently used settings, press the button “Save settings”, which is found under the Instrument menu in the main window. This brings up the dialog shown in Figure 52, in which it is possible to inspect the parameter setup that will be saved and to specify a name for these settings. It is highly recommended that you give the parameter setup a descriptive and easily remembered name.

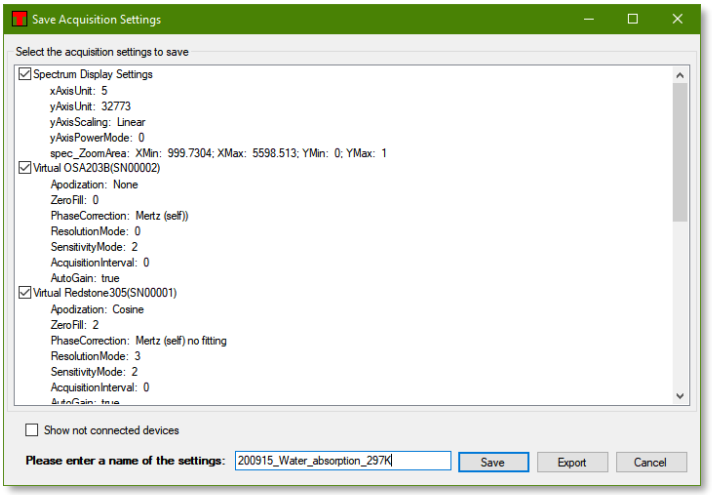


Figure 52. Save Acquisition Settings Dialog, Storing Settings to File for Later Use

Saved Settings can be Restored in Three Ways:

1. Clicking on the small arrow next to the button “Load Settings”, found under the Instrument menu in the main window, brings up a list of the names of previously saved setups. Clicking on one of these names will instantly load these settings and apply them. Please allow a few seconds for the settings to fully apply.

2. Clicking on the “Load Settings” button will bring up the “Load Acquisition Settings” dialog (see Figure 53). This allows for the inspection of the settings behind a saved name before loading the settings. It is also possible to rename or delete a stored parameter setting from the menu that is displayed when right clicking on any element on the list.

3. Clicking a Trace Label to open the Trace Options menu, and select “Revert Instrument to These Settings” found under the Settings sub-menu. This will change the acquisition settings to the ones used to capture that trace. To find out which settings will be loaded, open the Trace info window, also found under the Trace Options menu.

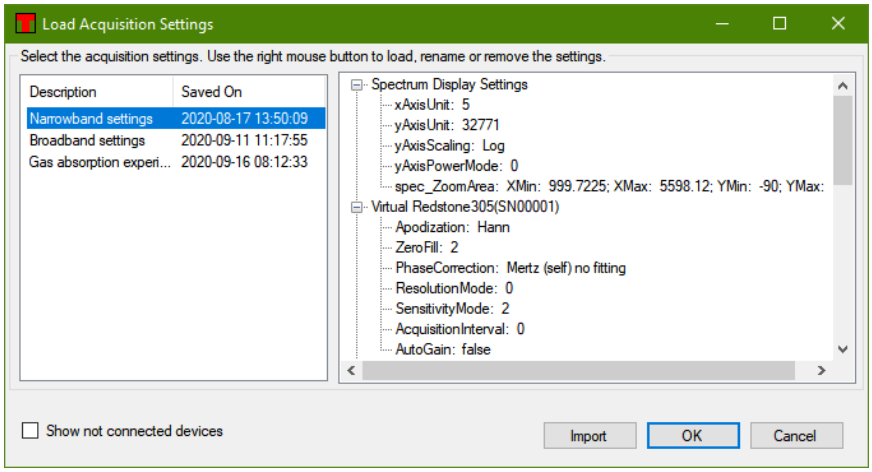


Figure 53. Load Acquisition Settings Dialog

Chapter 5 Virtual Instruments

The ThorSpectra software can be used without a spectrometer connected to the PC through the use of virtual instruments. A virtual instrument is a simulation of an instrument and allows for getting a feeling for the capabilities of the instrument and the software without the need for a real device.

To setup a virtual instrument, start the ThorSpectra software and open the Devices dialog by pressing the button “Devices” found in the Instrument menu. In the Devices dialog, press the button “Virtual.” This will bring up a dialog, in which the virtual instrument can be configured. Start by selecting the type of instrument that you wish to simulate by selecting one of the device types in the list to the left. Then select the type of source that you wish to simulate by selecting one of the source types in the list to the right. Clicking “Add” will then create the virtual device and add it to the list of instruments displayed in the Devices dialog.

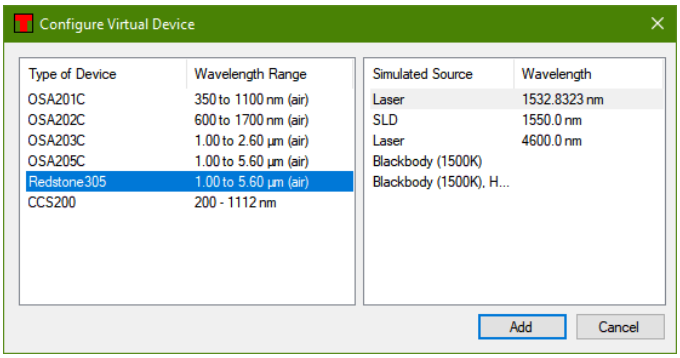
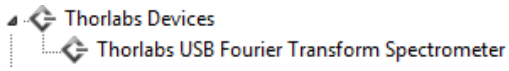


Figure 54. Virtual Devices Dialog

Once the virtual instrument is setup it can be operated in the same way as a regular Thorlabs instrument, for instance, press the button “Repeat” or “Single” to acquire spectra from the instrument.

To remove the virtual instrument, press the “Connect Devices” button or restart the software.

Chapter 6 Troubleshooting

Problem	Action
Software installation failed	Be sure to have administrative rights on your computer which enables you to install the software. Ask your system administrator to give you such rights or to do the installation.
ThorSpectra software cannot find any instrument	If the instrument was connected after the ThorSpectra software was started, it will not automatically detect the instrument. Press the button "Connect Devices" found under Instrument menu to search for connected instruments, see Section 3.3.1 Finding the Spectrometer. Check that Windows® has detected the instrument by opening the "Device manager" found under the Windows® Control panel. The instrument will be presented under the item "Thorlabs devices," as shown below. Note that it might be necessary to select "Show hidden devices." If Windows® has not detected the instrument, please make sure that the instrument is turned on and connected to the PC with a USB cable verified for the instrument type. If no instrument is found, check the connection of the USB cable or reboot the instrument. 
I have started the measurement, but the screen doesn't update	Start by checking your settings: • Make sure at least one trace is set to "Write" or "Average", see Section 3.6.2 Trace Update Options. • Certain combinations of settings have a very slow update rate, especially High Resolution/High Sensitivity. Please check the green progress bar in the bottom left corner. If the bar is visible, the device is still acquiring or processing data. • Is the acquisition interval set to anything other than zero milliseconds? This setting is found in the Settings dialog under the tab "Acquisition" (you might need to switch to "Advanced level" in the Settings dialog to see this). The acquisition interval is the minimum time between two data acquisitions. • If the interferogram is saturated or non-linear, the data will not be shown and a new acquisition is automatically requested. Open the Signal window from the Instrument menu and make sure that the gain is set to Automatic so that the Autogain algorithm can find optimal settings.
I cannot change the vertical or horizontal axis of the data display	Check if the axis is locked. This is done by clicking on the axis itself. If the check box "Lock axis" is checked, the displayed data range on that axis cannot be changed. This is to prevent accidental dragging or right-clicking in the graph to change the data range displayed. Simply uncheck the "Lock axis" check box and click "Ok." See the description found under Section 3.2 Customizing the Display.
If all else fails	Bring up the Error log by simultaneously clicking Ctrl+Shift+E. Save it to file and attach it to an email to **techsupport@thorlabs.com**.

Chapter 7 Thorlabs Worldwide Contacts

For technical support or sales inquiries, please visit us at **https://www.thorlabs.com/locations** for our most up-to-date contact information.



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