TII Spectrometry

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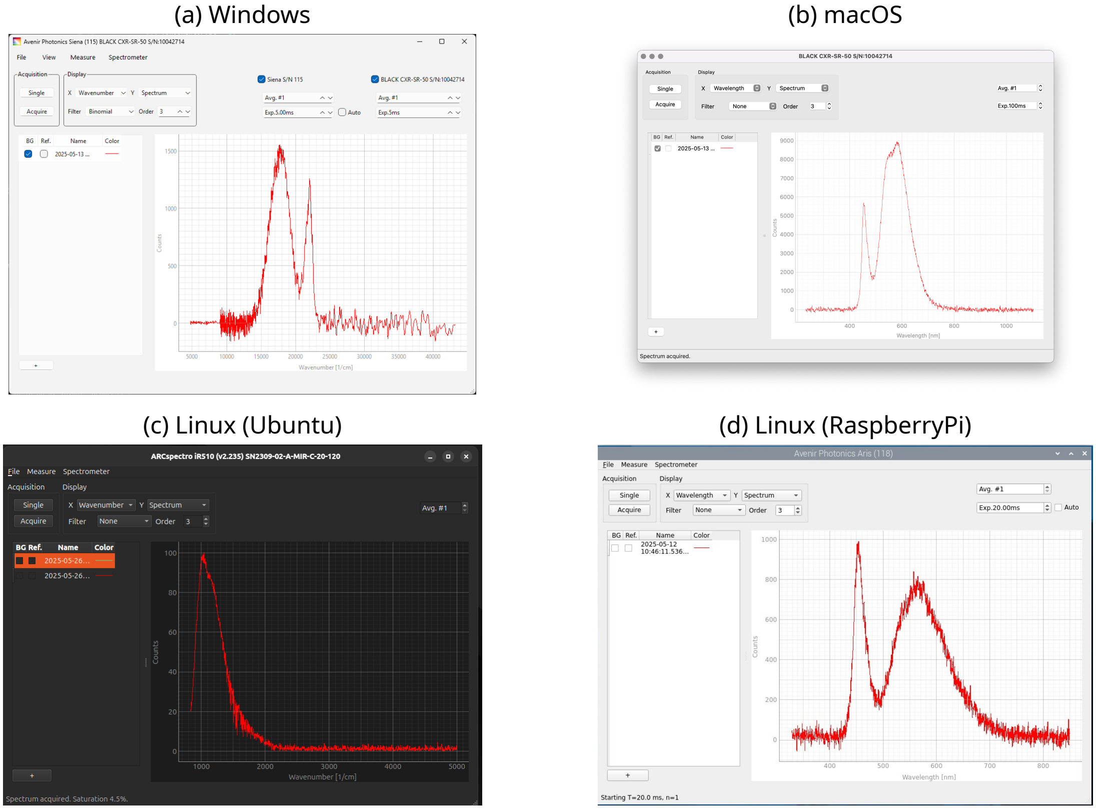
CHAPTER

ONE

INSTALLATION



(a) Windows

(b) macOS

(c) Linux (Ubuntu)

(d) Linux (RaspberryPi)

Fig. 1.1: **TII Spectrometry** on different platforms.

TII Spectrometry is a cross-platform application to control integrated visible or infrared light spectrometers and analyze the acquired spectra. Installation of the software differs by platform:

- on *Windows*, simply copy the **TII Spectrometry** folder to any desired location and double-click on `TII-Spectrometry.exe`
- on *macOS*, drag the `TII-Spectrometry` bundle to the `Applications` folder. The app can be opened by double-clicking `TII-Spectrometry`
- on *Linux* navigate to the folder containing the `TII-Spectrometry.deb` file and execute `sudo dpkg -i TII-Spectrometry.deb`. This will add **TII Spectrometry** to the desktop menu.

ℹ **Note**

The `TII-Spectrometry.deb` contains `*.rules` files to grant USB access to **TII Spectrometry**, which will be installed to `/etc/udev/rules.d/` using the above command. A reboot or log-in / log-out cycle may be required to gain access to USB devices after the first installation.

1.1 Supported Devices & Environments

TII Spectrometry supports the *Windows*, *macOS* (Apple Silicon) and *Linux* operating environments. On *Linux*, both *x64* (i.e. desktop computers) and *arm64* (e.g. RaspberryPi single-board computers) are supported. Most spectrometers are supported on all platforms, see Table 1.1 for exceptions. *Simultaneous control of multiple supported spectrometers* (page 17) is supported.

Table 1.1: Supported Devices & Environments

	Windows	macOS	Linux (x64)	Linux (arm64)
Avenir[2]	✓	✓	✓	✓
StellarNet[3]	✓	✓	✓	✓
NLIR Midwave[4]	✓	✓	✓	✓
ARCoptix FTIR[5]	✓		✓[6]	✓

[2] https://www.avenirphotonics.com/

[3] https://www.stellarnet.us/

[4] https://nlir.com/

[5] https://arcoptix.com/

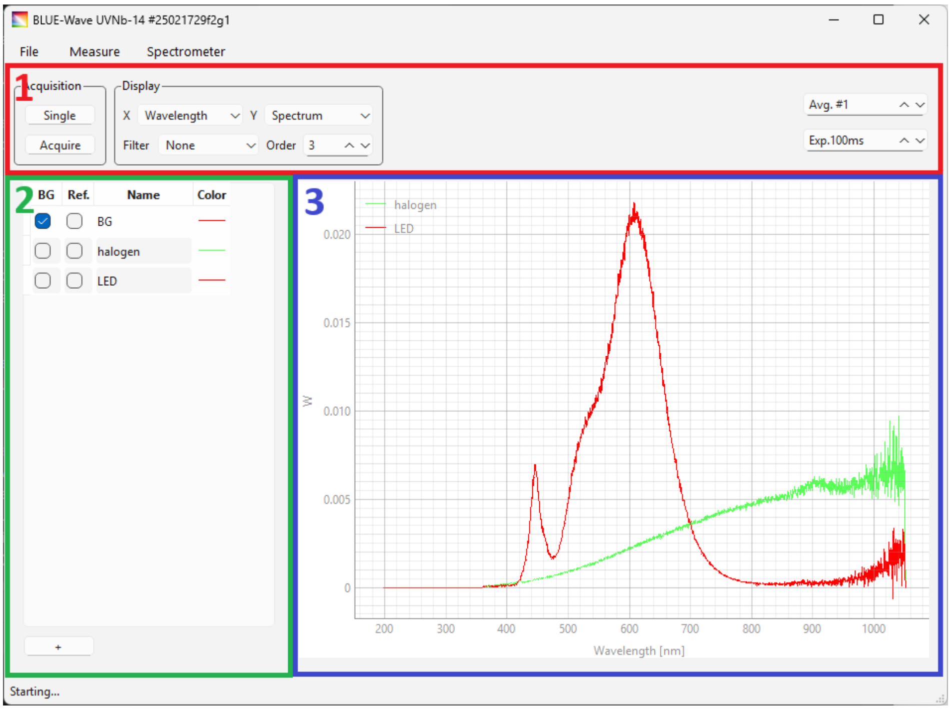
[6] Requires Ubuntu 22 (Jammy Jellyfish)

RECORDING SPECTRA

This section describes the operation of single or multiple connected spectrometers controlled by **TII Spectrometry**. Section 2.1 describes the features common to all spectrometers, Section 2.2 has additional information specific to particular spectrometers, and Section 2.3 describes how to control multiple spectrometers simultaneously. Section 2.4 contains information on how to acquire spectral time-lapse recordings.

2.1 General Use

This section describes how to acquire single spectra using **TII Spectrometry**.



BLUE-Wave UVNb-14 #25021729f2g1

X Wavelength Y Spectrum

Filter None Order 3

Avg. #1

Exp.100ms

BG	Ref.	Name	Color
☑	□	BG	🟥
□	□	halogen	🟩
□	□	LED	🟥

Starting...

Fig. 2.1: The **TII Spectrometry** user interface.

The main window of **TII Spectrometry** is divided into three sections:

1. The *top bar* (page 4) (red box in Figure 2.1) configures spectral acquisition an display
2. the *sidebar* (page 6) (green box in Figure 2.1) contains saved spectra and allows selecting *background and reference spectra* (page 7)
3. The *spectrum view* (page 7) (blue box in Figure 2.1) contains one or more spectra.

2.1.1 Connection

To connect to a spectrometer, use any of the following methods:

- select *File* ‣ *Connect* ‣ *Connect*. This will connect to the first detected spectrometer.
- select *File* ‣ *Connect* ‣ *Device Manager* to open the *Device Manager* and select the desired spectrometer(s) from the list. For details see the section *Using Multiple Spectrometers* (page 17).
- open a *device configuration file* (page 5) using *File* ‣ *Connect* ‣ *Load Configuration*. This will connect to the spectrometers in the configuration file if they are connected to the computer.

If the connection was successful, the connected spectrometer(s) will be displayed in the title bar of the **TII Spectrometry** window and the *Single* and *Acquire* buttons become active (Figure 2.1).

2.1.2 Device Configuration

The top bar of the **TII Spectrometry** window (red box in Figure 2.1) allows the configuration of the most relevant experimental parameters:

Spectral Acquisition

Single
Acquires a single spectrum using the current configuration

Acquire
Starts the spectrometer and continuously acquires spectra. Clicking the *Stop* button stops continuous acquisition.

Avg. #
Selects the number of spectra to average. Use this to improve the signal-to-noise ratio

Exposure Time
The exposure time of the detector in milli-seconds.

See also

Averaging and exposure time can be set individually for each connected spectrometer, see section *Using Multiple Spectrometers* (page 17) for details.

Display

This section allows to change how spectra are displayed in the spectrum view (blue box in Figure 2.1).

X
Selects the spectral domain:

- wavelength in *nm*
- wavenumber in *1/cm*

Y
Selects what parameter to display on the vertical axis:

- *Spectrum* displays the spectrometer counts. If a *background spectrum* (page 7) has been recorded, it is subtracted before display.
- *Absorbance* computes an absorbance spectrum $A = -\log_{10}\frac{I}{I_0}$, where I_0 is a *reference spectrum* (page 7)
- *Transmittance* computes an transmittance spectrum $T = \frac{I}{I_0}$, where I_0 is a *reference spectrum* (page 7)

> **Note**
>
> The *Absorbance* and *Transmittance* mode require a *reference spectrum* (page 7).

Filter

Activates spectral post-processing to reduce noise (Figure 2.2). Available filters are:

- *None*: No filtering, the spectrum is left untouched.
- *Moving Avg.*: A *moving average*[7] filter.
- *Binomial*: A binomial (Gaussian)[8] filter.

Order

Selects the window size of the moving average of binomial filter (Figure 2.2).

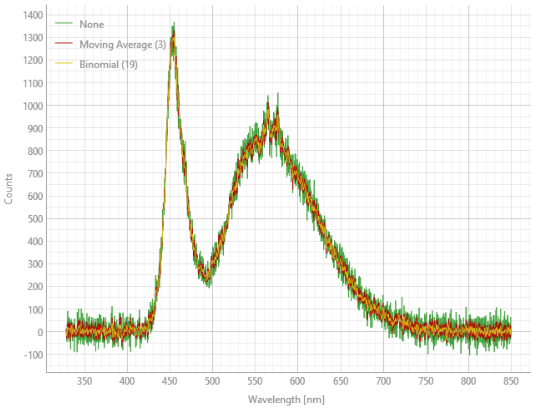


Fig. 2.2: Effect of *Filter* and *Order*.

Device Configuration Files

Device configuration (including *multiple spectrometers* (page 17)) can be saved to disk using *File* ‣ *Save Configuration*. Configuration files include:

- the connected spectrometers
- *exposure parameters* (page 4)
- *intensity calibrations* (page 9)
- external triggering (if supported)
- various *device-dependent parameters* (page 12)

To load a configuration file, use *File* ‣ *Connect* ‣ *Load Configuration*. An example configuration file is displayed *below* (page 5).

```
{
    "spectrometers": [
        {
            "n_average": 1,
            "spectral_domain": 1,
            "intensity_calibration": [

            ],
            "use_intensity_calibration": false,
```

(continues on next page)

[7] https://en.wikipedia.org/wiki/Moving_average

[8] https://en.wikipedia.org/wiki/Gaussian_filter

(continued from previous page)

```
                "intensity_calibration_unit": "W",
                "identifier": "Aris S/N 118",
                "use_nlir": false,
                "use_nlir_crop": true,
                "exposure_time": 1.0,
                "gain": 0,
                "external_trigger": false,
                "manufacturer": "Avenir"
            }
        ]
}
```

Note

Background and reference spectra (page 7) are not saved in the device configuration but can be saved and loaded from disk using the *save dialogue* (page 11) and saving in the `.hdf5` format.

2.1.3 Recording Spectra

To record a single spectrum, click *Single* in the *top bar* (page 4). To continuously acquire spectra, click *Acquire*, to stop spectral acquisition, click *Stop*.

Warning

Spectra will not be saved during continuous acquisition. To acquire spectra continously at regular time intervals, use a *time-lapse acquisition* (page 19).

2.1.4 Saving Spectra

To save the currently displayed spectrum, click the + button at the bottom of the sidebar. This will add the spectrum to the sidebar. In the sidebar, you can:

- select several spectra (using `Ctrl+Click` or `Shift+Click`) to display in the spectrum view, e.g. for comparison
- change the name of a spectrum by `double-clicking` on the spectrum's name
- change the spectrum's color by `double-clicking` on the color
- delete spectra by
  - pressing the `Delete` key
  - `right-clicking` on the selected spectra and selecting *Delete* from the context menu
- reorder spectra using drag&drop
- copy the selected spectra's data to the system clipboard in the `.csv` format using *Copy* or `Control-C`
- duplicate spectra by selecting *Duplicate* from the context menu
- reprocess spectra selecting *Reprocess* from the context menu

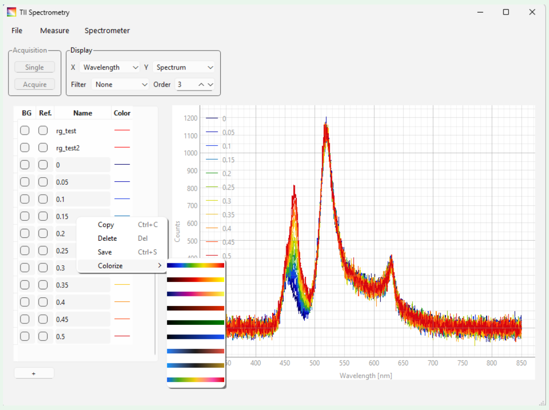
Note

Saved spectra are immutable. To change a spectrum, e.g. using *filtering* (page 5), *background subtraction* (page 7) or by *changing its spectral domain* (page 4), select *Reprocess* from the context menu. To perform reprocessing on a copy (to leave the original spectrum untouched), select *Duplicate* followed by *Reprocess*.

To save the selected spectra, select *Save* from the context menu. See the section *File Input & Output* (page 11) for details. To select all spectra, use `Control-A`.

Hint

If more than two spectra are selected, the *Colorize* option will become available. This allows applying a color scale to differentiate the selected spectra, which can be useful to highlight spectral differences of spectra acquired under different conditions (Figure 2.3)



X: Wavelength; Y: Spectrum
Filter: None; Order: 3

BG	Ref.	Name	Color
□	□	rg_test	🟥
□	□	rg_test2	🟥
□	□	0	🟦
□	□	0.05	🟦
□	□	0.1	🟦
□	□	0.15	🟦
□	□	0.2	
□	□	0.25	
□	□	0.3	
□	□	0.35	🟨
□	□	0.4	🟧
□	□	0.45	🟥
□	□	0.5	🟥

Fig. 2.3: Colorizing Traces

Background & Reference Spectra

- to select a saved spectrum as the *background spectrum*, check the *BG* column in the *spectra sidebar* (page 6). The intensity values of the background spectrum will be subtracted from all subsequent recorded spectra.
- to select a saved spectrum as the *reference spectrum*, check the *Ref.* column in the *spectra sidebar* (page 6). This will enable Absorbance (page 4) and Transmittance (page 4) calculations.

Tip

Meaningful background and reference spectra have to be acquired under experimental conditions similar to the acquat spectral recordings, e.g. using the same exposure time and illumination. To improve the signal-to-noise ratio of background or reference spectra for subsequent calculations:

- use *averaging* (page 4) during recording
- use *filtering* (page 5) to reduce noise by post-processing.

2.1.5 Spectrum Display

The spectrum view (blue box in Figure 2.1) displays one or more selected spectra. The view can be adjusted

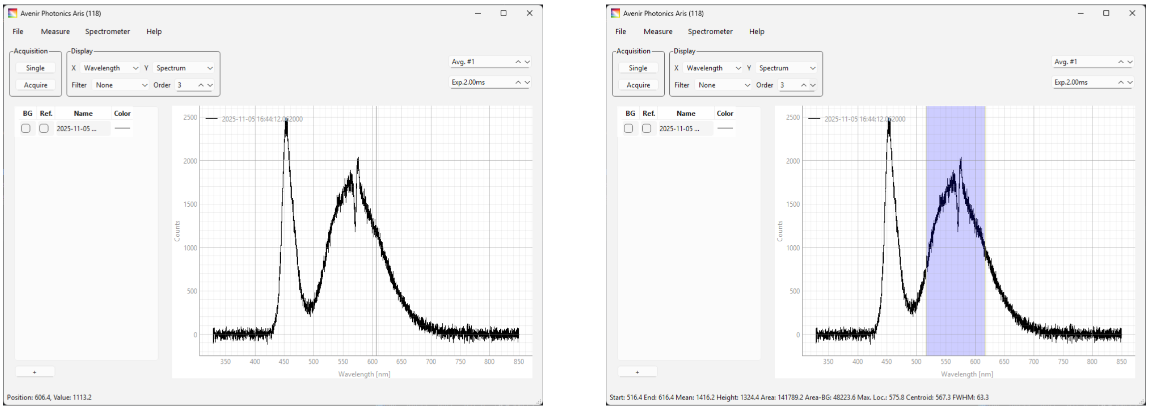
- using the scroll wheel to zoom
- dragging while holding down the right mouse button to zoom

- dragging while holding down the left mouse button to pan

To reset the display (autoscaling all traces)< click the *A* button at the bottom left corner.

Additionally, the context menu (`right-click`) offers the following options:

- *View All*: autoscales the view
- *X Axis* and *Y Axis* adjust the visible X and Y range ad allow autoscaling one axis only
- *Cursor*. Displays a cursor or region-of-interest selector
  - the *Cursor* (*Cursor* ‣ *Cursor*) is a vertical bar that can be dragged using the mouse. The position of the cursor (x value) and the spectral intensity at the selected position (y value) are displayed at the bottom of the **TII Spectrometry** window (Figure 2.4).
  - the *region-of-interest (ROI) selector* (*Cursor* ‣ *Region*) marks a region that can be dragged and resized using the mouse. Various parameters of the selected region are displayed at the bottom of the **TII Spectrometry** window (Figure 2.4). For details on how the parameters are computed, see Section 3.1.


(a) Cursor

(b) ROI

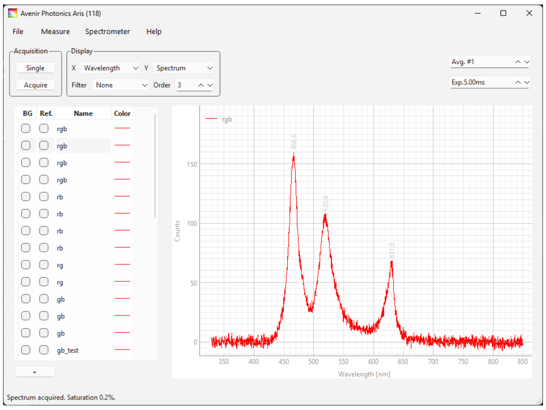
X Wavelength, Y Spectrum, Filter None, Order 3, Avg. #1, Exp.2.00ms

Position: 606.4, Value: 1113.2

Start: 516.4 End: 616.4 Mean: 1416.2 Height: 1324.4 Area: 141789.2 Area-BG: 48223.6 Max. Loc.: 575.8 Centroid: 567.3 FWHM: 63.3

Fig. 2.4: Spectrum View - Cursor Display

- *Show Peaks* toggles peak position display in the spectrum view (Figure 2.5)

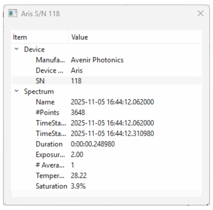

X Wavelength, Y Spectrum, Filter None, Order 3, Avg. #1, Exp.5.00ms

BG	Ref.	Name	Color
□	□	rgb	—
□	□	rgb	—
□	□	rgb	—
□	□	rgb	—
□	□	rb	—
□	□	rb	—
□	□	rb	—
□	□	rb	—
□	□	rg	—
□	□	rg	—
□	□	gb	—
□	□	gb	—
□	□	gb	—
□	□	gb_test	—

Spectrum acquired. Saturation 0.2%.

Fig. 2.5: Peak Display

- *Acquisition Parameters* displays the *Acquisition Parameters* window (Figure 2.6), which contains metadata of the acquired spectrum.



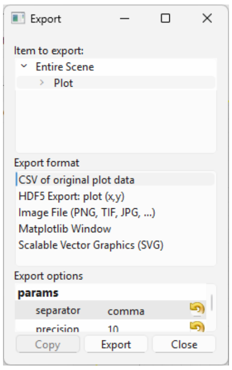
Aris S/N 118

Item	Value
Device	
Manufa...	Avenir Photonics
Device ...	Aris
SN	118
Spectrum	
Name	2025-11-05 16:44:12.062000
#Points	3648
TimeSta...	2025-11-05 16:44:12.062000
TimeSta...	2025-11-05 16:44:12.310980
Duration	0:00:00.248980
Exposur...	2.00
# Avera...	1
Temper...	28.22
Saturation	3.9%

Fig. 2.6: The Acquisition Parameters Window.

- *Export* displays the *Export Dialog* window (Figure 2.7). This window allows:
  - the export of the plot as an image
  - the export of the plot's underlying data as `.csv` or `.hdf5`

  to disk or the system clipboard.



Export

Item to export:

Entire Scene

Plot

Export format

CSV of original plot data

HDF5 Export: plot (x,y)

Image File (PNG, TIF, JPG, ...)

Matplotlib Window

Scalable Vector Graphics (SVG)

Export options

params

separator comma

precision 10

Fig. 2.7: The Export Dialogue Window

Hint

The spectrum view graph can also be copied to the system clipboard using standard system commands (e.g. `Control-C` on Windows).

Important

The `.hdf5` files exported using the *Export Dialogue* cannot be re-imported into **TII Spectrometry**. For round-tripping, use the *Save command* (page 7) in the *spectrum sidebar* (page 6).

2.1.6 Intensity Calibration

Intensity calibration describes the process of using a spectrum of a reference light source with a a known intensity distribution (typically a black-body emitter with a well-characterized color temperature) to correct the sensitivity and throughput of the spectrometer and input optics at different wavelengths. If the radiance or irradiance of the light source are known, recorded spectra can, in addition, be made fully quantitative, which is essential for many applications of *radiometry* (page 29). To calibrate a spectrometer:

1. record a spectrum of the reference light source (using appropriate *acquisition settings* (page 4) and, if required, *background subtraction* (page 7))

> **Important**
>
> Since the calibration curve will be calculated by division using the intensity of the reference lightsource and the reference spectrum, a high signal-to-noise ratio of the calibration spectrum is advisable.

2. select *Spectrometer* ‣ *Intensity Calibration* ‣ *Calibrate* to display the calibration window (Figure 2.8)

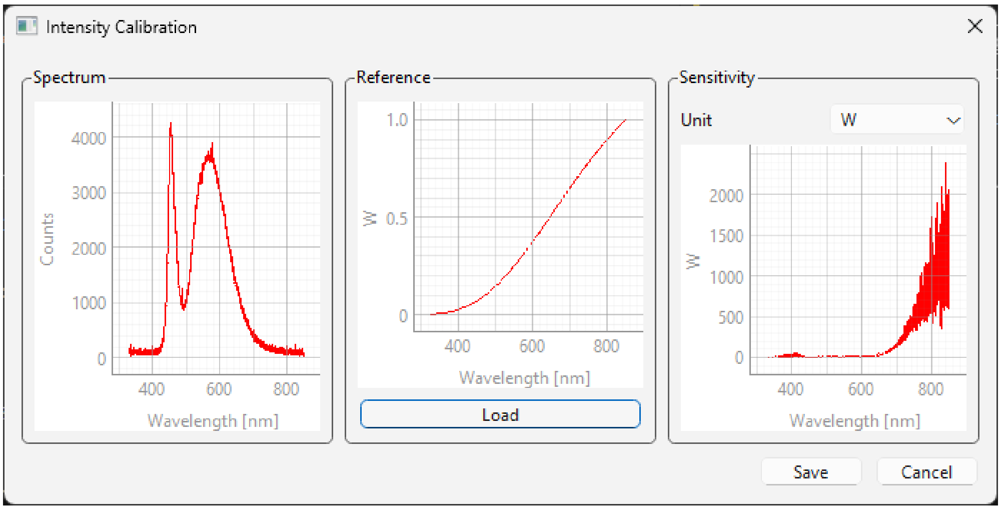


Fig. 2.8: The Calibration Window

3. The spectrum of the reference light source is displayed in the left-most graph. To load the reference intensity data, click the *Load* button and select the reference data

> **Important**
>
> - reference data is expected to be in a two-column `.csv` format (Listing 2.1) with no header.
>
>   Listing 2.1: Sample calibration data
>
>   ```
>   193.00  0.0000E+000
>   193.50  0.0000E+000
>   194.00  0.0000E+000
>   ```
>
>   Here,
>
>   - the first column contains the wavelength in *nanometers* or wavenumber in *1/cm*
>   - the second column contains the reference value of the light source, e.g. spectral power in *W*.
>
> - the spectral range of the reference data is expected to match (or exceed) the spectral range of the recorded reference spectrum. This means that the spectral domain (wavelength or wavenumber) has to match as well
> - the reference data will be interpolated to match the sampled wavelengths of the recorded spectrum

4. The reference intensity data will be displayed in the center graph.
5. Select the unit of the reference intensity

6. The calibration curve (sensitivity curve) will be displayed in the right-most graph
7. Click *Save* to accept the calibration.

> **Note**
>
> The sensitivity curve is normalized by the exposure time. This means the exposure time can be varied during subsequent spectral acquisitions to achieve the desired signal-to-noise ratio or to avoid saturating the detector...

To use the intensity calibration, check *Spectrometer ‣ Intensity Calibration ‣ Apply*. The intensity calibration will be applied to subsequently recorded spectra.

> **Hint**
>
> Calibration data can be saved in a *device configuration file* (page 5) so this procedure only has to be reperformed if the optical setup changes.

> **See also**
>
> See the appliction example *The Solar Spectrum* (page 47) for additional hints and information.

2.1.7 File Input & Output

Spectral data can be exported from **TII Spectrometry** in a variety of ways:

- selecting one or more spectra in the *spectrum sidebar* (page 6) and selecting *Copy* from the context menu (or using the shortcut `Control`-C) copies the spectral data to the system clipboard using the `.csv` format. This allows direct pasting into third-party graphing or analysis software.
- selecting one or more spectra in the *spectrum sidebar* (page 6) and selecting *Save* from the context menu (or using the shortcut `Control`-S) displays a file dialogue and allows saving the spectral data to disk. Available formats are `.csv` and `.hdf5`.
  - `.csv`[9] files enjoy widespread support and can be imported by virtually all third-party software
  - `.hdf5`[10] files are the native file format of **TII Spectrometry** and can be re-imported for later analysis. These files can be read using a wide variety of applications including MATLAB[11], Igor Pro[12], and Origin Pro[13]. Python support is available via the h5py[14] package. In addition to the wavelength and intensity data, this format also contains
    - raw intensity values (before background subtraction etc.)
    - timestamps
    - additional metadata

  > **Tip**
  >
  > A convenient way to inspect `.hdf5` files is the https://myhdf5.hdfgroup.org/ website.

[9] https://en.wikipedia.org/wiki/Comma-separated_values
[10] https://en.wikipedia.org/wiki/Hierarchical_Data_Format
[11] https://www.mathworks.com/products/matlab.html
[12] https://www.wavemetrics.com/products/igorpro
[13] https://www.originlab.com/
[14] https://docs.h5py.org/en/stable/

- using the Export Dialogue (page 9) in the spectrum view.

Note

The recommended output format is `.hdf5` exported from the *spectrum sidebar* (page 6), which retains most information.

To re-import `.hdf5` data into **TII Spectrometry**,

- use *File* ‣ *Load Data* and select a `.hdf5` file from the file dialogue
- drag and drop one or more `.hdf5` files onto the spectral sidebar

2.2 Supported Devices

This section contains information on specific spectrometers supported by **TII Spectrometry**. For guidance on general use common to all supported devices, see Section 2.1.

Important

Not all spectrometers are supported on all platforms. For details, see Table 1.1.

2.2.1 Avenir Photonics

TII Spectrometry supports the Avenir Photonics[15] *Aris* (visible) and *Siena* (near-IR) spectrometers. In addition to the *standard spectrometer settings* (page 4), the following settings are available in the *Spectrometer* menu:

LED
Toggles the spectrometer's LED

Auto
Activates auto-exposure mode

External Trigger
Activates external triggering

Gain
(Avenir *Siena* only) sets the gain

NLIR
activates *NLIR Spectrum upconverter* (page 16) support

In addition, the *Burst Time-lapse Recording* (page 22) window contains the following settings:

Data Format
Changes the data format of the spectrometer for higher throughput.

- *32bit float*
- *16bit Int*
- *16bit Int (Half Spectral Resolution)*

The default (*32bit float*) has the highest resolution and fidelity. To increase the spectral acquisition rate and to avoid filling up the spectrometer's internal buffer, a more compact data format (*16bit Int* or *16bit Int (Half Spectral Resolution)*) can be selected. The effect of this setting can be seen in Figure 2.9: When using the *32bit float* format (blue), the spectrometer buffer fills up after approximately 180 spectra and the spectral acquisition rate slows down

[15] https://www.avenirphotonics.com/

from 250 Hz to 125 Hz. For the *16bit Int (Half Spectral Resolution)* setting (red & green), the spectrometer can continuously operate at full speed.

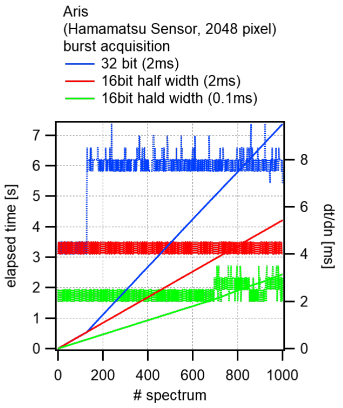


Fig. 2.9: Sustained spectral acquisition rate of an Avenir *Aris* spectrometer

2.2.2 ARCoptix

TII Spectrometry supports ARCoptix[16] FTIR (FT-NIR and FT-MIR) spectrometers. Theses devices are based on a scanning Michelson interferometer and cover spectral ranges in the near and mid infra-red.

Note

ARCoptix spectrometers rely on a serverlet application that runs in the background. If the application is not already running, it will be started by **TII Spectrometry**. The initialization of this application as well as connection to and configuration of the spectrometer can take several 10s of seconds. In principle, connection to the serverlet application is also possible using over a network connection - see the section *Remote Connections* (page 15) for details.

Important

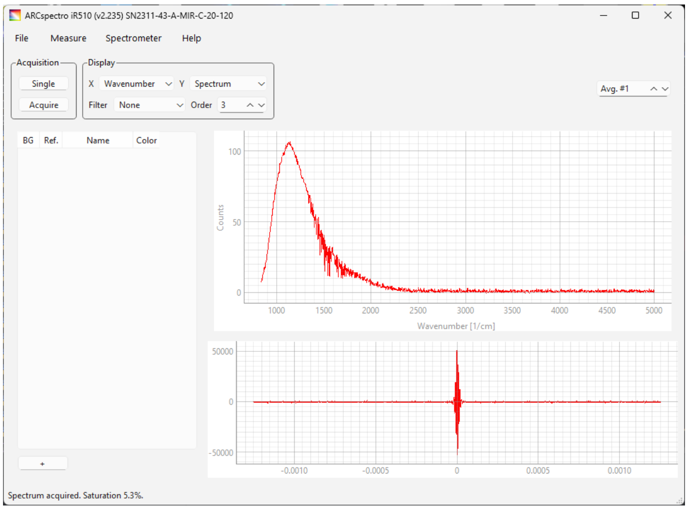
Since the scan rate of the interferometer is fixed, no exposure time settings are available.

The *Spectrometer* menu contains the following options:

Apodization
Selects an apodization function[17] to remove high-frequency noise at the expense of a reduced spectral resolution

Interferogram
Toggles the display of the raw interferogram data (bottom of Figure 2.10).

[16] https://arcoptix.com/Spectrometers.htm
[17] https://en.wikipedia.org/wiki/Apodization



ARCspectro iR510 (v2.235) SN2311-43-A-MIR-C-20-120

X Wavenumber Y Spectrum

Filter None Order 3

Avg. #1

Spectrum acquired. Saturation 5.3%.

Fig. 2.10: The interferogram view

See also

See Section 5.1 (*Fast Fourier Transform (FFT) Applied to FTIR Data* (page 61)) for guidance on how to analyze interferogram data.

Gain

Selects the gain of the spectrometer

Resolution

Selects the spectral resolution in *1/m*. Higher numbers increase the scan speed but lower the spectral resolution by decreasing the scan range of the interferometer (Figure 2.11).

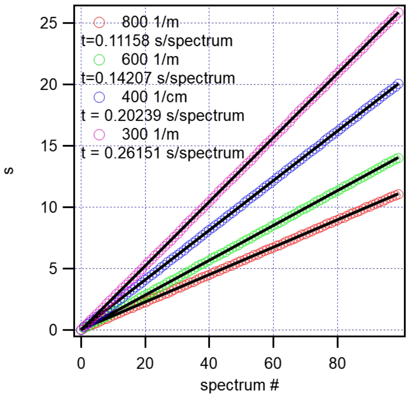


Fig. 2.11: Spectral acquisition rate vs resolution

Warning

Changing the spectrometer resolution will reconfigure and disconnect the spectrometer from **TII Spectrometry**. To continue using the spectrometer, simply *connect again* (page 4).

Remote Connections

Connections to the ARCoptix serverlet applications are possible over a network connection provided the computer running the serverlet application (*'host'*) and the computer running **TII Spectrometry** (*'guest'*) are part of the same subnet.

To establish a network connection:

1. on the *host* computer:
   - connect the spectrometer to a USB port
   - start the serverlet application:
     - on Windows, this is done by starting `AoDAQWin.exe`
     - on Linux, this is done by running `AoDAQ_**`, where `**` indicates the suffix for the file version and operating system

   > **Tip**
   >
   > Use `AoDAQWin.exe -h` (on Windows) for help. It may be helpful to:
   >
   > - run the application in *verbose mode* using `AoDAQWin.exe -v` for troubleshooting
   > - manually set a port number for the TCP/IP connection using, e.g. `AoDAQWin.exe -p 4711`

2. on the *guest* computer:
   - start **TII Spectrometry**
   - open the Device Manager (page 18) using *File ‣ Connect ‣ Device Manager*
   - enter the IP address and port number of the host computer and activate the *ARCoptix (remote)* device

     > **Tip**
     >
     > The default port number is 1424.

   - click *OK* to establish the connection

> **Note**
>
> Remote and local spectrometers can be mixed - see Section 2.3 *Using Multiple Spectrometers* (page 17) for details.

2.2.3 StellarNet

TII Spectrometry supports StellarNet[18] spectrometers. In addition to *standard spectrometer settings* (page 4), the following settings are available in the *Spectrometer* menu:

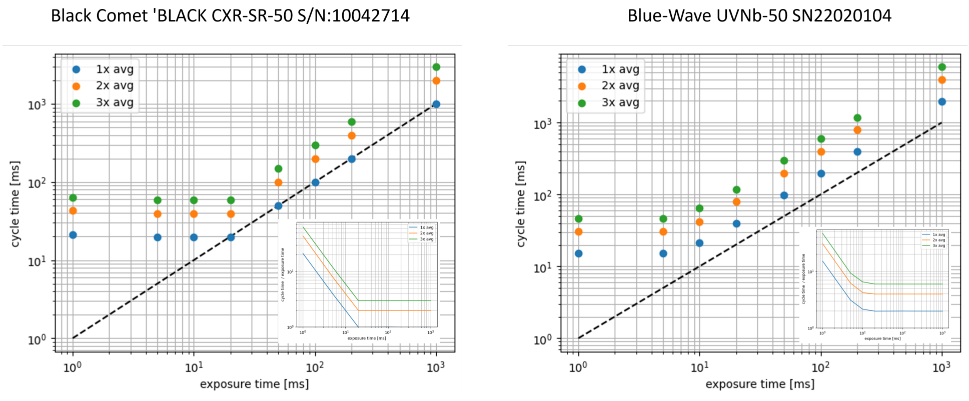
X-Timing
Sets the X-timing

Temperature Compensation
Toggles temperature compensation using dark pixels to increase spectrometer stability during long recordings.

[18] https://www.stellarnet.us/

NLIR

activates *NLIR Spectrum upconverter* (page 16) support


Black Comet 'BLACK CXR-SR-50 S/N:10042714

Blue-Wave UVNb-50 SN22020104

Fig. 2.12: StellarNet spectrometer timing

2.2.4 NLIR Spectrum

The NLIR Spectrum[19] is a wavelength converter that uses sum-frequency generation (SFG) of a 1064 nm laser (λ_{pump}) with mid-infrared light (λ_{MIR}) in a non-linear crystal for spectral upconversion of the 1900-5300 nm mid-IR spectral range to the 682-886 nm visible range (λ_{NIR}) (2.1).

$$\frac{1}{\lambda_{\text{NIR}}} = \frac{1}{\lambda_{\text{MIR}}} + \frac{1}{\lambda_{\text{pump}}} \tag{2.1}$$

This device can be connected to supported spectrometers for recording MIR spectra using a VIS-NIR device. The NLIR Spectrum is supported if the spectral range of the connected spectrometer includes the output range of the upconverter (682-886 nm). In this case, the *Spectrometer* menu will include the *Spectrometer ‣ NLIR* submenu.

Use

Toggles spectral re-conversion using (2.1) solving for λ_{MIR}. The spectral axis will hence be in units of the original mid-IR light before upconversion.

Crop

Removes the spectral region outside of the upconversion output range.

The effect of these two settings is displayed in Figure 2.13: The bottom axis shows the wavelength of the upconverted spectrum, the top axis shows the wavelength of the original light before upconversion. The green region marks the spectral range of the wavelength converter - spectra will be cropped to this region if *Crop* is enabled.

[19] https://nlir.com/products/wavelength-converters/spektrum/

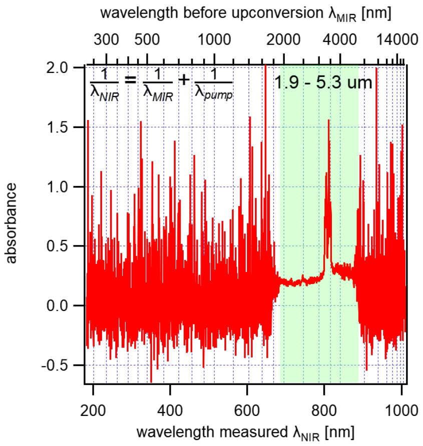


Fig. 2.13: Spectral output of the NLIR Spectrum wavelength converter

2.2.5 NLIR Midwave

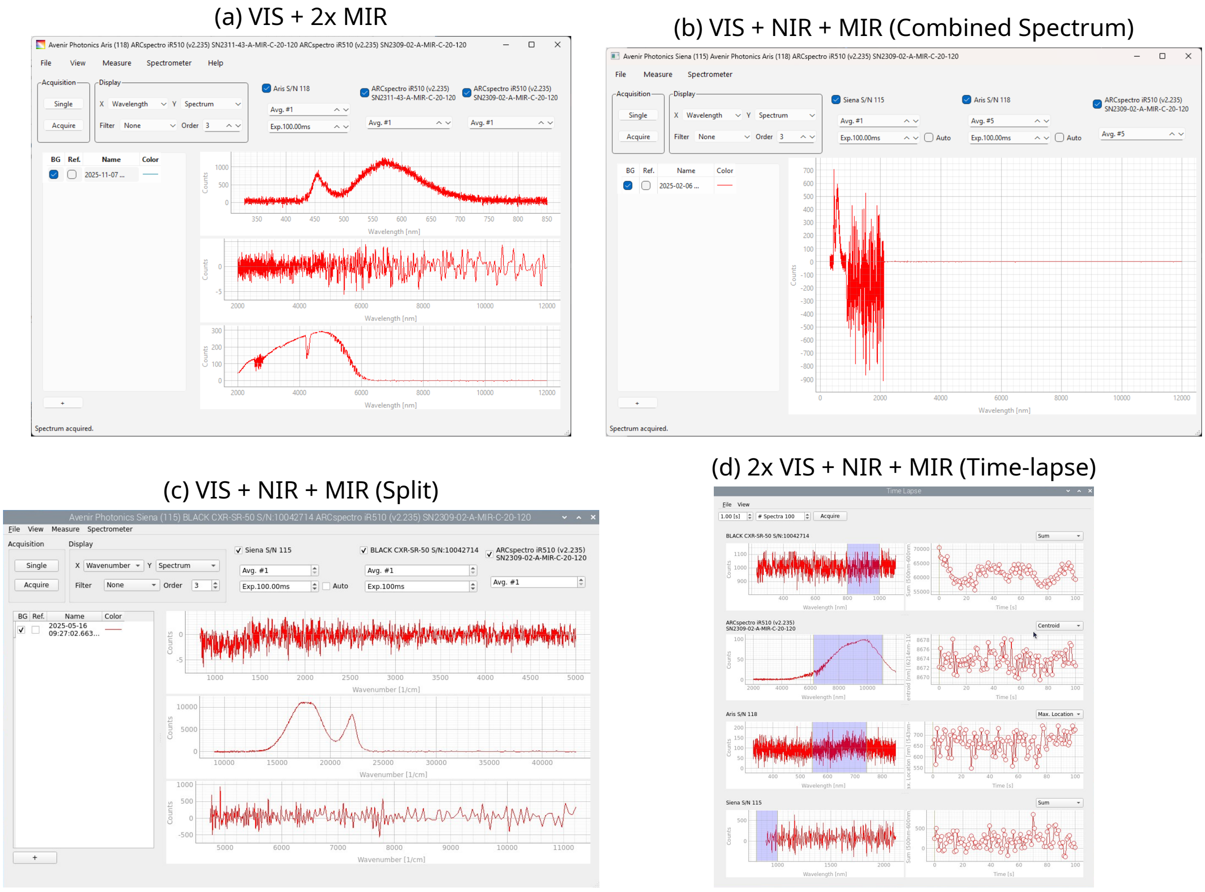
The NLIR Midwave[20] is a combination of *NLIR spectral upconverter* (page 16) and spectrometer. In addition to *standard spectrometer settings* (page 4), this device also allows external triggering, which can be activated using *Spectrometer ‣ External Trigger ‣ Use External Trigger*. The trigger edge (rising or falling) can be selected using *Spectrometer ‣ External Trigger ‣ Trigger Edge*. Spectra are automatically re-converted to the MIR range.

2.3 Using Multiple Spectrometers

TII Spectrometry supports the simultaneous control of multiple supported spectrometers . This can be useful in the following scenarios:

- to combine spectrometers monitoring a single source with adjacent spectral ranges to expand spectral coverage. This used in the application example 'The Solar Spectrum *(page 47)*'
- to use multiple spectrometers (with identical or different spectral coverage) to monitor several processes simultaneously

[20] https://nlir.com/products/spectrometers/midwave/



(a) VIS + 2x MIR

(b) VIS + NIR + MIR (Combined Spectrum)

(c) VIS + NIR + MIR (Split)

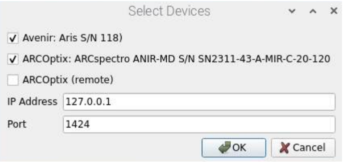
(d) 2x VIS + NIR + MIR (Time-lapse)

Fig. 2.14: Using multiple spectrometers in **TII Spectrometry**

Examples for these applications are displayed in Figure 2.14. There are *no limitations* on the number or type of spectrometers that can be controlled simultaneously in **TII Spectrometry**.

> **See also**
>
> See Table 1.1 for supported devices on different platforms and Section 2.2 for caveats applying to individual device classes.

2.3.1 Device Manager



Select Devices

☑ Avenir: Aris S/N 118)

☑ ARCOptix: ARCspectro ANIR-MD S/N SN2311-43-A-MIR-C-20-120

□ ARCOptix (remote)

IP Address 127.0.0.1

Port 1424

Fig. 2.15: The *Device Manager*

To connect to *multiple* spectrometers, use the *Device Manager* (Figure 2.15), which can be accessed using *File* ‣ *Connect* ‣ *Device Manager*. The *Device Manager* window will display all supported and connected devices. To connect:

- enable the checkbox for the devices you would like to connect to
- click *OK*

See also

See Section 2.2.2 for details on *remote connections to ARCoptix devices* (page 15).

2.3.2 Use & Display Options

Connected devices will be displayed on the *top bar* (page 4) of the main window. Here:

- you can set the exposure time and averaging number for each device device individually
- use the checkbox to activate or (temporarily) deactivate one or more devices.

Two display options are available:

- the *Combined* view. Here, spectra from different devices are combined and displayed on the same spectral axis. This is useful when using multiple spectrometers to expand spectral coverage.
- the *Split* view. Spectra are displayed in separated graphs.

> **See also**
>
> Figure 2.14 shows examples for these two display modes.

- The *Measure* menu gives access to Time-lapse Recordings (page 20), which allows software-synchronized time-lapse acquisitions using multiple spectrometers. In the Time-Lapse *window* (page 20), you can switch between *Combined* and *Split* display using the *View* menu.
- The *Spectrometer* menu gives access to spectrometer settings for each connected device, e.g Intensity Calibration (page 9)
- recordings using multiple spectrometers can be *processed* (page 7), *saved* (page 6), and *loaded* (page 11) from disk just like regular, single-device spectra.
- *multi-spectrometer configurations* (page 5) can be saved and reloaded.

2.4 Time-Lapse Recordings

In time-lapse recordings, spectra are recorded at regular intervals, e.g. to monitor a chemical reaction. **TII Spectrometry** supports two time-lapse modalities:

1. regular *time-lapse* (page 20). Here, timing is controlled by the host PC and spectra are acquired at a regular, user-defined interval. This mode

   - supports software synchronization of *multiple spectrometers* (page 17) (Figure 2.16).
   - spectra are updated in real time

   On the other hand, this mode is unsuitable for high spectral acquisition rates and the software-based timing makes some timing jitter unavoidable.

   > **Note**
   >
   > While the maximum throughput of the regular time-lapse mode depends on the connection speed, CPU load and other factors, a good role of thumb is that the maximum rate will be around 20Hz.

   Time-lapse mode can be accessed using *Measure ‣ Time Lapse*, which shows the *time lapse window* (page 21).

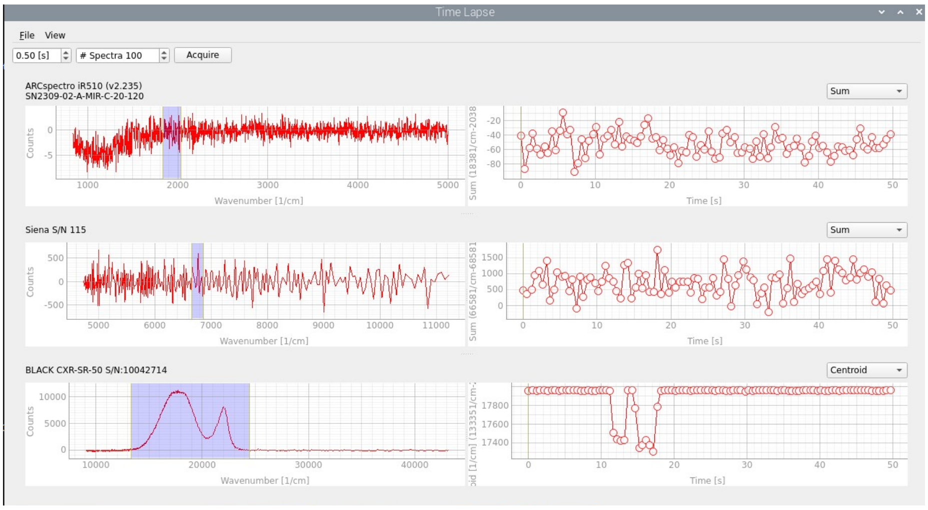


Fig. 2.16: Time-lapse recording using multiple spectrometers

2. *burst time-lapse recordings* (page 22). Here,
   - only a single spectrometer is supported
   - graphical display is delayed or disabled until the recording is complete
   - timing is left up to the spectrometer hardware
   - if supported, spectra are buffered in spectrometer memory and read in bulk

   This mode supports very fast acquisition rates > 1000 Hz (depending on spectrometer support). Burst recordings can be accessed using *Measure ‣ Burst Acquisition*

Note

Burst acquisitions are only available on selected spectrometers (Table 2.1)

Table 2.1: Burst Mode Availability

Avenir	StellarNet	NLIR Midwave	ARCoptix
✓		✓	

Hint

Both time-lapse acquisition modes are compatible with external triggering (provided the spectrometer supports this) to carefully control timing and synchronization to an external signal. In this case, the expected spectral interval (exposure time or cycle time) should be smaller than the trigger interval.

2.4.1 Time-Lapse

Conventional time-lapse recordings can be accessed using *Measure ‣ Time Lapse*. In the *time-lapse window* (page 21), the following parameters can be configured:

Interval Time
The time interval (in *seconds* between spectral acquisitions). This should be longer than the exposure time (multiplied by the number of averages).

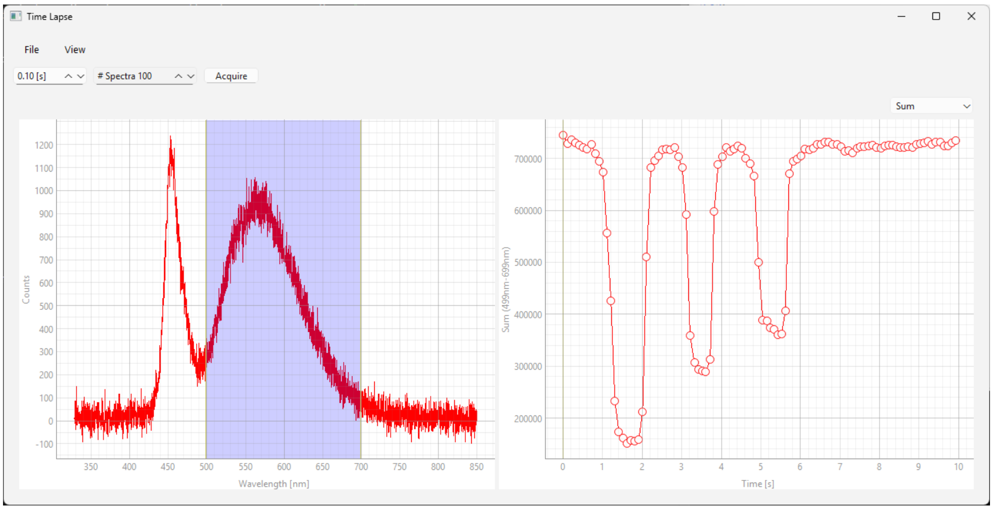
# of Spectra
The number of spectra to acquire

Hint

Other parameters can be configured in the main window. This includes

- *acquistion parameters* (page 4) (exposure time, averaging)
- *display and post-processing parameters* (page 4)

The *Acquire* button starts the time-lapse acquisition, which can be aborted by pressing the *Stop* button.



0.10 [s]

Spectra 100

Sum

Fig. 2.17: The time-lapse window

In the time-lapse window (Figuee 2.17), the left pan contains the current spectrum. The right graph contains a plot of a selected spectral parameter vs the acquisition time.

- the region of interest (blue box in the left graph) can be moved and resized using the mouse.
- the currently displayed spectrum can be selected by dragging the vertical marker in the right graph
- the displayed parameter can be selected using the drop-down menu at the top right

> **See also**
>
> Please see the *section on time-lapse analysis* (page 23) for further details on parameter computation.

- if multiple spectrometers are connected and active, a pair of spectrum and time-lapse graphs is displayed for each spectrometer, see Figure 2.16 for an example.

Time-lapse recordings can be saved to disk using *File* ‣ *Save*. Available formats are `.csv` and `.hdf5`. Time-lapse recordings saved in the `.hdf5` can be re-imported using *File* ‣ *Load* for further analysis in **TII Spectrometry**.

Note

The listing below displays an example time-lapse `.csv` file.

Listing 2.2: The time-lapse `.csv` format

```
            ,         0.0,          0.1,          0.2,          0.3
328.385131836,-22.7980957031,38.7015953064,5.24367284775,32.3832092285
328.552246094,30.9543762207,14.3859844208,0.124359227717,89.9606399536
```

- the first row contains the timestamps in *seconds*.
- the first column contains the wavelength / wavenumbers
- the remaining columns contain the spectral intensity

2.4.2 Burst Recordings

For supported spectrometers, burst acquisitions can be accessed using *Measure ‣ Burst Acquisition*. In the *burst acquisition window* (page 22), the following parameters can be configured:

Delay Time

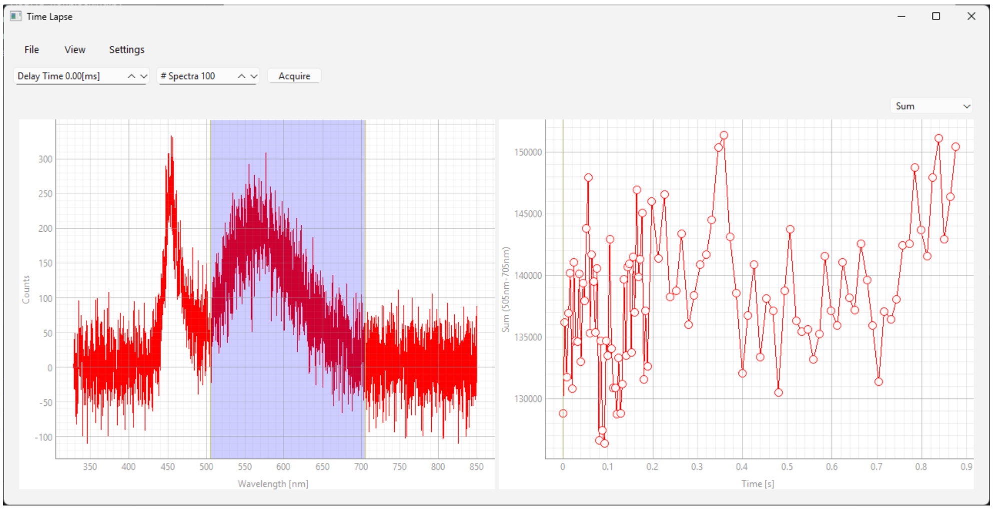
Configures an additional wait time (in *milli-seconds*) between exposures. The cycle time is the sum of the delay time and the exposure + readout time. When external triggering is used, the delay time is the delay between the trigger and the start of the exposure.

# Spectra

The number of spectra to record

As in software-controlled time-lapse recordings, other parameters can be *configured in the main window* (page 4).

The *Acquire* button starts the time-lapse acquisition, which can be aborted by pressing the *Stop* button.



Delay Time 0.00[ms]

Spectra 100

Fig. 2.18: The burst acquistion window

The *Settings* menu gives access to the following options:

Settings ‣ Update Graph

When unchecked (the default), the display is only updated once the acquisition is completed. If checked, graphs are updated at regular intervals (but not in real time).

Additional *spectrometer-specific settings* (page 12) also appear in the *Settings* menu.

Adjusting the displayed data, saving, and loading data is performed in the same fashion as for *conventional time-lapse recordings* (page 21).

CHAPTER

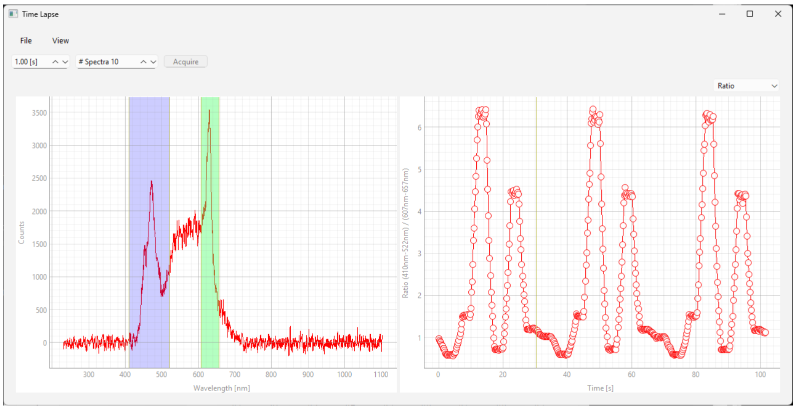
THREE

ANALYSIS

3.1 Time-Lapse Analysis

Time-lapse analysis allows the visualization of the evolution of spectral parameters vs time. Available parameters are:

- *Sum*: a running sum of the selected spectral region $I = \sum_{x_0}^{x_1} I_x$
- *Integral*: the area under the curve of the selected region (computed by trapezoidal integration) $I = \int_{x_0}^{x_1} I_x dx$. The difference to the *Sum* parameter is that the integral accounts for the (potentially non-constant) spacing of the data points.
- *Integral - BG*: The area under the curve of the selected region after subtraction of the baseline. The baseline is computed as the line connecting the borders x_0 and x_1 of the selected region.
- *Height*: The difference between the minimum and maximum intensity of the selected region.
- *Max. Location*: The location (in units of wavelengths / wavenumber) of the point with the highest intensity.
- *Centroid*: computes the centroid (center of mass) of the peak in the selected spectral region. For symmetric peaks, this is equal to the peak's location, i.e. its highest value. Unlike *Max. Location*, *Centroid* can interpolate the location and thus compute peak positions at a resolution higher than the spectral resolution of the data. The center of mass is defined as: $x_{\mathrm{COM}} = \frac{\sum x_i I_i}{\sum I_i}$.
- *FWHM*: The full width at half maximum of the selected region.
- *Ratio*: The integrated intensity ratio of two selected regions (blue and green regions in Figure 3.1)



1.00 [s]

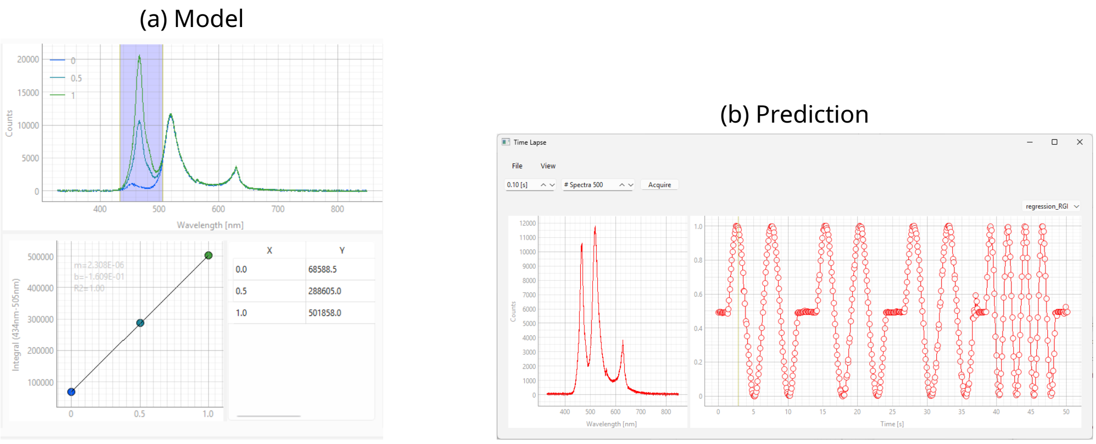
Spectra 10

Ratio

Fig. 3.1: Peak ratio analysis

- *Ratio - BG*: The integrated intensity ratio of two selected regions after subtracting the baseline.

- *Load Model*: Loads a *pre-trained regression model* (page 38) and uses this model to extract a numerical value (e.g. a concentration based on a calibration curve) from the spectra (Figure 3.2). Several models can be loaded. Models appear in the menu using their file name.


(a) Model

(b) Prediction

X	Y
0.0	68588.5
0.5	288605.0
1.0	501858.0

Fig. 3.2: Timelapse regression analysis

Hint

Time traces can be exported by `right-clicking` on the (right) time trace view and selecting *Export* to show the *Export dialogue* (page 9).

3.1.1 The Time-Lapse Analysis Window

The time-lapse analysis window can be accessed via *View* ‣ *Analysis* in the *time-lapse window* (page 23). The analysis window has three panes:

1. the spectral image view (Figure 3.1). This view shows the acquired spectra as a spectral image, with the spectral dimension as the horizontal axis, the elapsed time as the vertical axis, and the spectral intensity as the image color.
   - the current spectrum (shown at the bottom) can be selected by dragging the vertical marker.
   - the spectral region of interest can be selected by moving and resizing the vertical rectangle.
   - the image color can be adjusted by dragging the markers in the top color scale

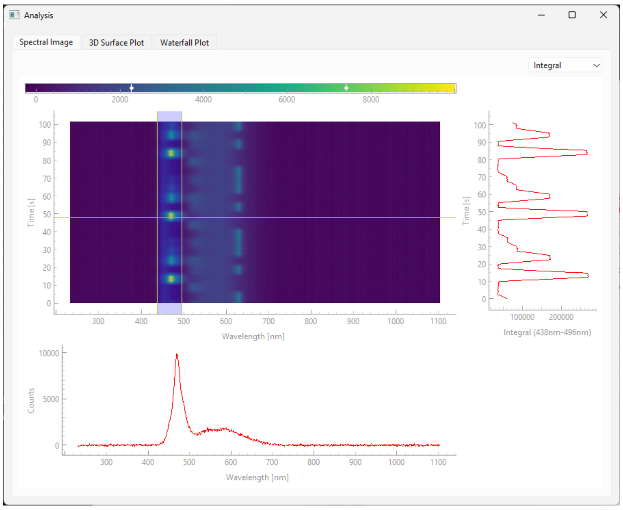


Fig. 3.3: Time-lapse Analysis - Spectral Image

The vertical graph on the left displays a time trace of the selected parameter, similar to the *time lapse window* (page 23).

2. the surface plot view (Figure 3.4). This shows a 3D representation of the time-lapse dataset that can be rotated and zoomed using the mouse.

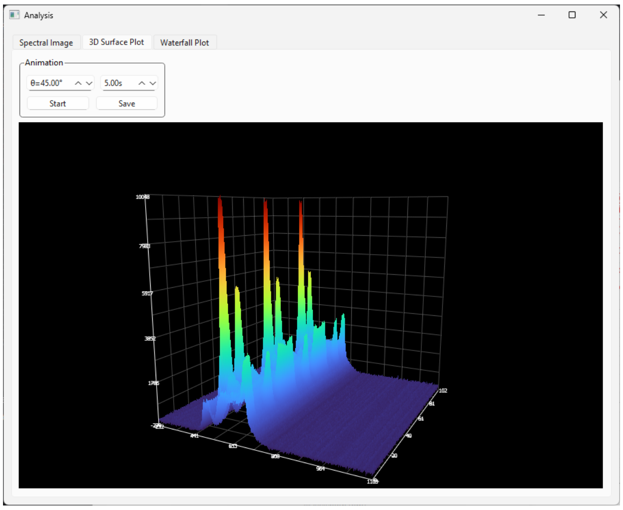
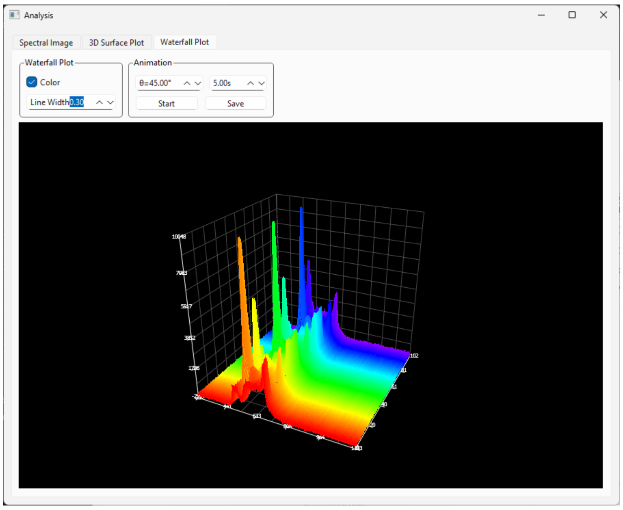


Fig. 3.4: Time-lapse Analysis - 3D surface

3. the waterfall plot view (Figure 3.5). This plot is more suitable for sparse time-lapse recordings with only few acquired spectra. The (optional) coloring indicates time (in contrast to the 3D surface plot where it represents intensity).



Waterfall Plot

☑ Color

Line Width 0.30

Animation

θ=45.00°

5.00s

Fig. 3.5: Time-lapse Analysis - Waterfall

Hint

The 3D surface and waterfall plots can be animated using the *Animation* settings box. Animations can be exported as `.gif` or .png using the *Save* button.

3.2 Colorimetry

Spectrophotometric *Colorimetry*[21] describes the interaction of light with a sample across the entire visible spectrum (typically 400 nm to 700 nm) to get a numerical representation of its color. *Colorimetry* is available for all spectrometers operating in the visible range and can be accessed using *Analysis* ‣ *Colorimetry* to show the *Colorimetry window* (Figure 3.6).

See also

See the application example *Colorimetry of Light Sources & Color Charts* (page 48) to see see colorimetry in action.

Colorimetric analysis performs the following steps:

- raw spectral data (a spectral reflectance curve for opaque solids or a spectral transmittance curve for transparent liquids/solids) is converted into colorimetric values that correspond to how the human eye perceives color under *specific lighting conditions* (page 28)
- the spectral curve data is mathematically integrated with *standard Observer functions* (page 28) (e.g., the CIE 1931 Standard Observer[22]) and standard Illuminant data (e.g., D65 for daylight) to calculate the X, Y, and Z tristimulus values. These values represent the perceived amount of Red, Green, and Blue light, respectively. The Tristimulus Values (X, Y, Z) are calculated by integrating the product of these three functions over the visible spectrum:

$$X = k \sum_{\lambda} R(\lambda) S(\lambda) \bar{x}(\lambda) \Delta\lambda$$

$$Y = k \sum_{\lambda} R(\lambda) S(\lambda) \bar{y}(\lambda) \Delta\lambda$$

[21] https://en.wikipedia.org/wiki/Colorimetry

[22] https://en.wikipedia.org/wiki/CIE_1931_color_space

$$Z = k \sum_{\lambda} R(\lambda) S(\lambda) \bar{z}(\lambda) \Delta\lambda$$

Where:

- $R(\lambda)$ is the measured spectral curve (from the spectrophotometer).
- $S(\lambda)$ is the SPD of the chosen illuminant.
- $\bar{x}, \bar{y}, \bar{z}$ are the CIE color matching functions.
- k is a normalizing constant.

The Y value is particularly important, as it represents the sample's absolute luminance or lightness.

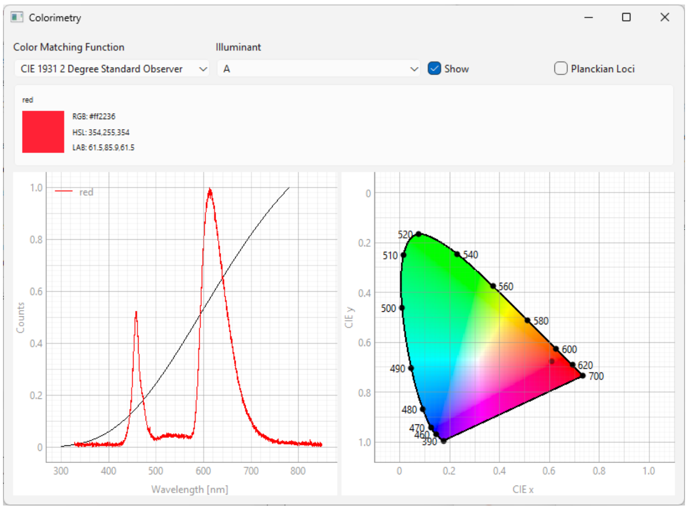
- The X, Y, Z values are converted into the two chromaticity coordinates (x and y) using ratios:

$$x = \frac{X}{X + Y + Z}$$

$$y = \frac{Y}{X + Y + Z}$$

and plotted in a chromaticity diagram (e.g. the CIE 1931 xy Chromaticity Diagram), a 2D projection that shows only the hue and saturation of a color, independent of its lightness (luminance) (Figure 3.6 right panel).

- The X, Y, Z values are transformed into coordinates in a uniform color space like the CIE $L^*a^*b^*$ (Lab) space.
  - L^*: Lightness (0=black, 100=white).
  - a^*: Red/Green axis (+a=red, -a=green).
  - b^*: Yellow/Blue axis (+b=yellow, -b=blue).
- The CIE X, Y, Z Tristimulus Values are converted to RGB (Red, Green, Blue) for display on a screen using the D65 white point.



Colorimetry

Color Matching Function: CIE 1931 2 Degree Standard Observer

Illuminant: A

☑ Show

□ Planckian Loci

red

RGB: #ff2236

HSL: 354,255,354

LAB: 61.5,85.9,61.5

Fig. 3.6: The *Colorimetry* window

The *Colorimetry* window is split into four sections (from top to bottom):

1. The top bar allows configuration of the *illuminant* (page 28) and *color matching function* (page 28) used in the analysis
2. the color result view, which contains:
   - a visual representation of the calculated color

- color values in the RBG, HSL, and CIE $L^*a^*b^*$ color space

Hint

Color values can be copied using drag & drop.

3. The spectrum view, which shows the selected spectrum and (optionally) the selected illuminant
4. the *chromaticity diagram* (page 27). The location of the selected spectrum in xy chromaticity coordinates will be indicated by a circle. The outline of the circle corresponds to the *color of the selected spectrum* (page 6).

Hint

Colorimetry works both in real time (live analysis while recording spectra) or post acquisition. To analyse saved spectra:

- display the *Colorimetry* window
- select the spectrum or spectra in the *spectrum side bar* (page 6)

Multiple spectra can be analyzed simultaneously (see Figure 4.6 for an example).

The *Colorimetry* window (Figure 3.6) gives access to the following settings:

Color Matching Function
Selects a standard observer function

Illuminant
Selects the illuminant, the light source that was used to record the spectrum. Illuminants include:

- standard incandescent illuminants with different color temperatures (A-D)
- fluorescent lamps
- LED illuminants

See also

See Figure 4.5 for an example of a LED illuminant.

Show
Toggles the display of the *selected illuminant* (page 28) spectrum in the spectrum plot (black trace in the left panel of Figure 3.6)

Planckian Loci
Toggles the display of Planckian Loci[23] (or Black Body Loci), a curved reference line in the *chromaticity diagram* (page 27). This line represents the color of an ideal black-body radiator as its temperature is increased from absolute zero up to infinity.

See also

See Section 3.3 on *Radiometry* (page 29) for more information, i.e. on the Correlated Color Temperature (CCT).

[23] https://en.wikipedia.org/wiki/Planckian_locus

3.3 Radiometry

Unlike Colorimetry (page 26), which deals with the analysis of colors that originate from the changes to the spectrum of a light source ('illuminant') by absorption or scattering of a sample, radiometry involves the characterization of the light source itself. The *Radiometry* window (Figure 3.7), which can be accessed using *Analysis* ‣ *Radiometry*, provides the following functionality:

- measurement of the physical energy emitted by a light source in Watts
- measurement of the *perceived brightness* (page 30) of visible light (Lumens). Here, we are taking radiometric data and weighting it according to the standardized human eye sensitivity curve[24] (V(λ)).

Important

For the computed values of energy or brightness to be physically meaningful, the spectrometer has to be calibrated using a light source with

- a known spectrum
- a known power output

To minimize geometric effects, the collection setup has to be carefully considered, for example by using an integrating sphere.

For qualitative comparison of light sources and their quality, omitting this calibration step is possible as long as the sensitivity curve of the spectrometer does not result in spectral distortion in the visible range.

- characterization of light source color rendering quality from the spectral power distribution (spectrum), e.g. *color temperature (CCT)* (page 32) or *color rendering index (CRI)* (page 32)

See also

See Section 4.3 - *Radiometric Analyis of Light Sources* (page 51) to see this in practice.

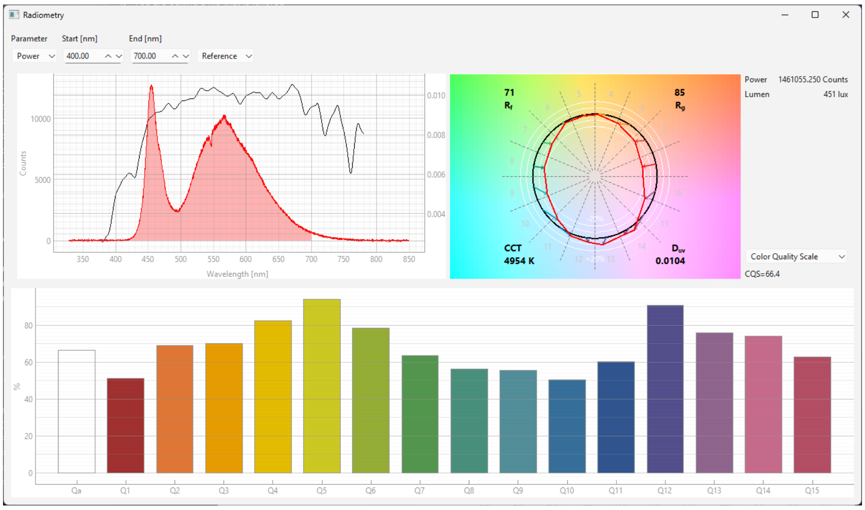

Parameter: Power
Start [nm]: 400.00
End [nm]: 700.00
Reference
Power 1461055.250 Counts
Lumen 451 lux
Color Quality Scale
CQS=66.4

Fig. 3.7: The *Radiometry* window

The *Ratiometry* window (Figure 3.7) hosts the following controls / UI elements (from top to bottom):

1. *the settings bar* (page 30)

[24] https://en.wikipedia.org/wiki/Luminous_efficiency_function

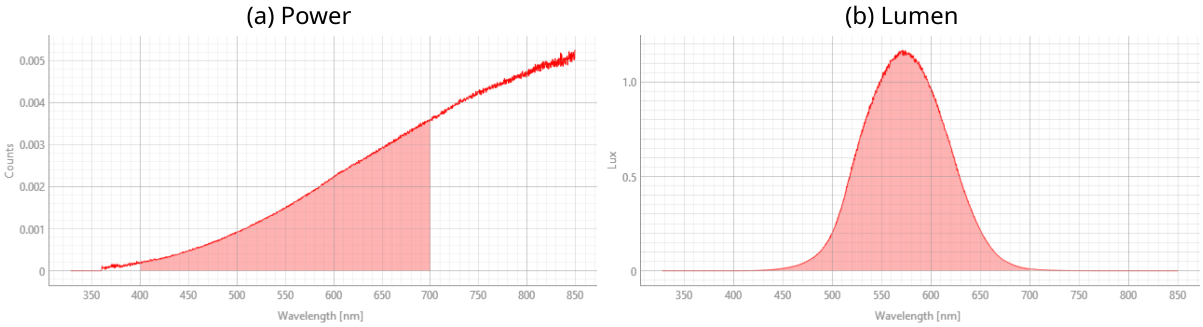
2. the spectrum view
3. *the Color Vector Graphic* (page 31)
4. *the result sidebar* (page 32)
5. *the quality metrics view* (page 32)

3.3.1 The Settings Bar

The *Settings* bar offers the following settings:

Parameter

switches between *Power* (emitted energy) and *Lux* (perceived brightness) (Figure 3.8). To compute the perceived brightness, the spectrum is multiplied by a standardized human eye sensitivity curve V(λ)[25], which is centered around 550 nm.



(a) Power

(b) Lumen

Fig. 3.8: Energy vs perceived brightness

Start

The lower spectral bound used to determine the emitted power

End

The upper spectral bound used to determine the emitted power

> **Hint**
>
> The area used for integration is indicated by the shaded region in the spectrum view.

Accessory Display

Toggles the (optional) display of either:

- the reference illuminant used for calculating the color fidelity index R_f and the color gamut index R_g. For a *color temperature (CCT)* (page 32) < 5000 K, a theoretical Planckian (black-body) radiator at that CCT will be used, for higher color temperatures, the CIE Daylight distribution will be used. See Figure 4.7 for further examples of reference illuminants.
- the raw spectral data (before intensity calibration)

> **Hint**
>
> Displaying the raw spectral data can be useful to judge how much of the dynamic range of the spectrometer is actually used and to optimize acquisition parameters to obtain a high-signal-to-noise ratio while avoiding saturating the detector.

[25] https://en.wikipedia.org/wiki/Luminous_efficiency_function

3.3.2 The IES TM-30-18 Color Vector Graphic

The *Color Vector Graphic* translates the numerical color quality data of a light source derived from its spectral power distribution (SPD) into a visual map of color shifts. The graphic is a circular plot that visually represents how a test light source changes the hue and saturation of colors compared to an ideal reference source (like daylight or a black-body radiator). It is divided into 16 hue bins (sections around the circle), which makes it easy to identify deficiencies or enhancements in specific color ranges (Figure 3.9).

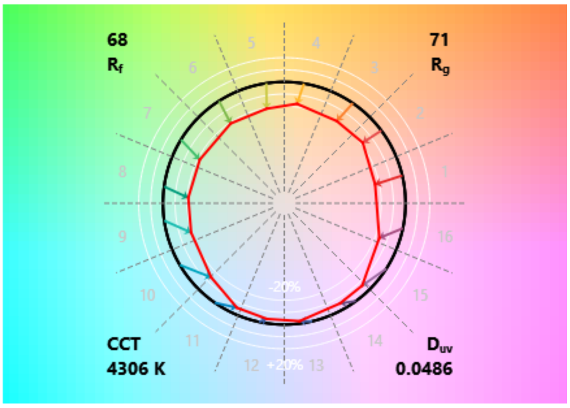


Fig. 3.9: The *Color Vector Graphic*

This plot shows:

The Reference Ring

The central black circle in Figure 3.9 represents the chromaticity coordinates of the 99 Test Color Samples (TCSs, also see Section 3.3.4) when illuminated by the reference source (the ideal source for that color temperature).

The Test Vector

The red line in Figure 3.9 shows the average chromaticity coordinates of the TCSs in each of the 16 hue bins when illuminated by the test light source.

By comparing the solid red line (test source) to the solid black line (reference source), one can determine the light source's local color rendering characteristics:

- Radial Distance (Saturation/Chroma Shift):
  - *Inward Shift*: If the red line falls inside the black circle, the test light source is desaturating (making duller) the colors in that specific hue bin.
  - *Outward Shift*: If the red line falls outside the black circle, the test light source is over-saturating (making more vivid) the colors in that hue bin. This shift is quantified by the Color Gamut Index (R_g), which gives the average saturation shift
- Tangential Distance (Hue Shift):
  - *Clockwise Shift*: The light source is shifting the perceived hue (the pure color) of objects in that bin towards the next color in the clockwise direction (e.g., from green toward yellow-green).
  - *Counter-Clockwise Shift*: The hue is being shifted towards the next color in the counter-clockwise direction.

    While there is no single hue-shift metric, this visual distortion is captured within the overall Color Fidelity Index (R_f) and the Local Color Fidelity ($R_{f,\text{hue}}$) for that bin.

In addition, the plot displays the following metrics:

***Color Fidelity Index*, R$_f$**

Measures the color accuracy or fidelity of the light source on a scale from 0 to 100. It tells us how closely the colors of objects will appear to their “true” color as seen under the reference light (usually daylight or a black-body radiator).

Color Gamut index, R$_g$

Measures the average increase or decrease in the saturation (chroma) of the colors rendered by the light source on a scale from 0 to 100. This metric is crucial because light sources, especially LEDs, can be designed to pump out intense light in specific wavelength bands (like red and green) to make colors “pop,” even if the fidelity ($\mathrm{R_f}$) isn’t perfect.

Correlated Color Temperature (CCT)

Indicates the color temperature of the light source in Kelvins (K). The *CCT* is calculated from the light source’s X, Y, Z tristimulus values, which are then used to determine its Correlated Color Temperature (CCT) from its position on the *chromaticity diagram* (page 27).

The $\mathrm{D_{uv}}$ Value

Quantifies a light source’s chromaticity offset from the Planckian Locus

- a positive $\mathrm{D_{uv}}$ indicates that the light source’s chromaticity is above the Planckian Locus. This results in a greenish or yellowish-green tint.
- a negative $\mathrm{D_{uv}}$ indicates that the light source’s chromaticity is below the Planckian Locus. This results a pinkish or magenta tint.

3.3.3 The Result Sidebar

The result section contains the calculated power and brightness. Here, you can also select which *color quality metric* (page 32) to compute:

- Color Rendering Index (CRI)
- Color Quality Scale (CQS)
- Color Fidelity Index (CFI)
- Local Color Fidelity
- Local Hue Shift
- Local Chroma Shift

Results for the selected metric will be displayed at the bottom in addition to updating the *test color sample graph* (page 33).

3.3.4 Color Quality Metrics

- *Color Rendering Index (CRI)*[26], R_α, a score between 0 and 100 that measures the light source’s ability to render colors accurately (Figure 3.10). The CRI is calculated using the *CIE 2024* standard. The R$_a$ score (General CRI) is based on the first eight samples (R$_1$ to R$_8$).

Note

While standard, CRI is known to have limitations, particularly for LED lighting with sharp spectral peaks, which can lead to a high CRI with poor appearance: A high R$_a$ value can be achieved even if the light source is poor at rendering certain saturated colors (especially deep red, R$_9$, which is not included in the R$_a$ average).

- *Color Quality Scale (CQS)*[27] (Figure 3.10). The *CQS* attempts to overcome limitations of the *CRI*, in particular the use of de-saturated test colors, which allowed LEDs with narrow spectral peaks (often missing deep reds) to score high while still rendering certain saturated colors poorly. *CQS* uses 15 saturated colors, ensuring the test light source is properly evaluated across the full color spectrum. The CQS is calculated using the *NIST CQS 9.0* standard.

[26] https://en.wikipedia.org/wiki/Color_rendering_index
[27] https://en.wikipedia.org/wiki/Color_quality_scale

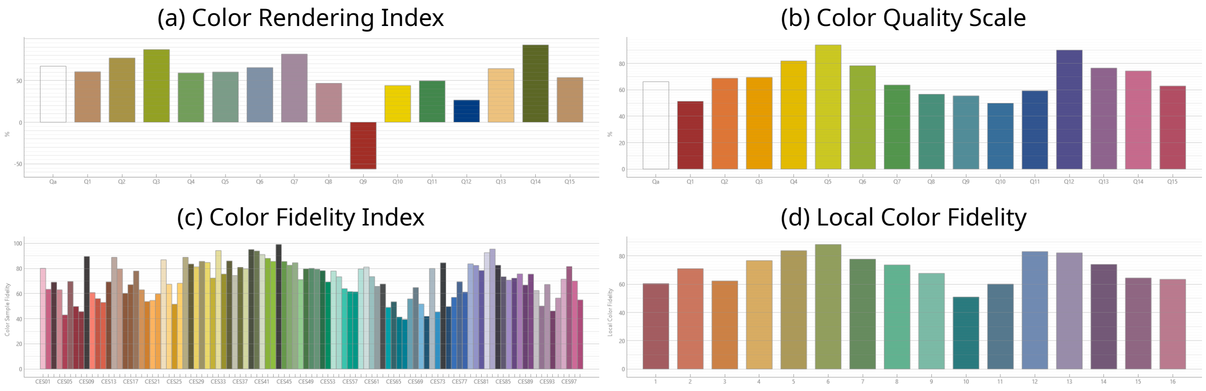
- the *IES TM-30-18 Color Fidelity Index (CFI)*[28] (Figure 3.10). This metric:
  - uses 99 test colors
  - separates fidelity (R_f) from gamut/saturation (R_g)

> **See also**
>
> The color vector graphic (page 31) is part of this analysis. Please see this section for a discussion of the parameters R_f and R_g.

- *Local Color Fidelity* (Figure 3.10), which compares the color fidelity accuracy across specific hue bins around the color wheel. The hue bins are the same as in the color vector graphic (page 31)
- *Local Hue Shift* and *Local Chroma Shift* reflect the hue / chroma differences compared to an ideal emitter and correspond to the direction / magnitude of the arrows in the color vector graphic (page 31).

The Test Color Sample Graph

The test color sample graph Figure 3.10 contains test color samples (TCS) in varying number and color depending on which color quality metric was selected. The color of each bar indicates the appearance of the test color sample as rendered considering the spectral distribution of the light source.



(a) Color Rendering Index

(b) Color Quality Scale

(c) Color Fidelity Index

(d) Local Color Fidelity

Fig. 3.10: Comparison of Color Rendering Metrics for the LED lightsource in Figure 3.7.

> **See also**
>
> The (as of late) free tool BabelColor[29] provides further radiometric analysis options.

3.4 Modeling

The *Modeling* package of **TII Spectrometry** allows to build and use predictive models to analyze spectral datasets. Taking spectra as the input, two different kinds of analysis are available:

- *Regression Analysis* (page 37): Regression is used when the output property you want to predict is a continuous numerical variable, for example concentration, quality score, temperature, or moisture level. A typical example would be concentration prediction by using the

[28] https://cie.co.at/publications/colour-fidelity-index-accurate-scientific-use
[29] https://babelcolor.com/index.htm

absorption spectrum of a chemical solution to predict the exact concentration of a solute, often relying on the Beer-Lambert Law[30].

- *Classification Analysis* (page 43): Classification is used when the output property you want to predict is a discrete, categorical label or class, such as material type, defect presence, or grade level. A typical example would be material identification: Classifying an unknown plastic sample as Polypropylene (PP) or Polyethylene (PE) based on its IR spectrum.

The *Modeling* package is can be accessed using *Analysis* ‣ *Modeling* ‣ *Train/Predict* and is available for any spectrometer.

See also

See the *Application Example Plastic Identification* (page 54) to see this in action.

3.4.1 General Overview

Details on Regression (page 37) and Classification (page 43) analysis will be discussed in dedicated sections.

Both types of analysis, however, share a common workflow:

1. record a *training* dataset, e.g. spectra of known materials (for *Classification*) or of known concentration (for *Regression*).
2. build a *Model* using this dataset (*Training*): This typically involves:
   - assigning labels (numerical or categorical) to the dataset
   - *preprocessing* (page 35) the data, e.g. by
     - Baseline Correction: Removing unwanted background signal offsets.
     - Normalization: Scaling the spectra to remove variations in overall light intensity or path length.
     - Smoothing: Reducing high-frequency noise.
     - Cropping: Remove unnecessary spectral regions.
   - training the model, e.g. using linear regression to fit a calibration curve
   - validating the model
3. once the *Model* has been trained, it can be used for *Prediction* using unknown samples. The model can also be saved to disk for later use.

Tip

Trained models can be used in **TII Spectrometry** in the following places:

- for real-time monitoring using both *Classification* and *Regression* models in the Monitor (page 44) view.
- to extract a numerical value from spectra (using a *Regression* model) during *time-lapse recordings* (page 23)

Note

In principle, *signals from more than one spectrometer* (page 17) can be incorporated into the model, e.g. spectrometers

[30] https://en.wikipedia.org/wiki/Beer%E2%80%93Lambert_law

- covering different spectral ranges
- spectrometers measuring the same process at different locations

Note

Models, are, at least in principle, device-independent, which means that models trained on spectral datasets of one spectrometer can be used for prediction using datasets of a different device. The following caveats apply:

- spectra have to appropriately normalized to account for differences in device sensitivity (this is best practice anyway)
- spectral ranges should (roughly) coincide and, crucially, include the spectral features that are required by the model for discrimination. As a trivial example, a model trained on near-IR data will (obviously) not work when using a spectrometer operating in the visible range. For spectral ranges of suitable overlap, **TII Spectrometry** will use interpolation and padding to transform spectral data and account for different spectral resolutions.

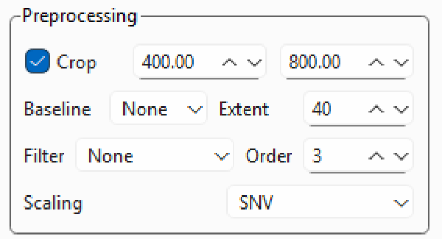
3.4.2 Pre-Processing

Pre-processing involves pre-treating the data to remove noise or scattering effects. Pre-processing options are shared between regression and classification models and the same rationale applies to both types of analysis.

Note

Pre-processing settings are part of the model. They will be saved in the model file and applied to spectra during the *Prediction* phase.

TII Spectrometry offers the following pre-processing settings (Figure 3.11):



Preprocessing

☑ Crop 400.00 800.00

Baseline None Extent 40

Filter None Order 3

Scaling SNV

Fig. 3.11: Pre-processing Settings

Crop
Allows selecting a spectral subregion.

Baseline
Removes a *non-linear* baseline from the dataset using the *Statistics-sensitive Non-linear Iterative Peak-clipping (SNIP)* algorithm (Ryan, 1988)[31]. The *Extent* parameter changes the curvature of the baseline.

Note

[31] https://doi.org/10.1016/0168-583X(88)90063-8

> A constant offset can easily be removed using *Scaling* (page 36). If the baseline can be removed by *background subtraction* (page 7) during spectral acquisition, this is likely preferable.

Filter

Applies a convolutional smoothing filter to the data. The settings are identical to the Filter *setting* (page 5) in the main window.

Scaling

Scales (normalizes) the data. Three options are available:

- *None*: Performs no scaling
- Min-Max (page 36): Scales each spectrum in the range between 0 and 1.
- *SNV*: Applies Standard Normal Variate *scaling* (page 36).

> **Important**
>
> Scaling is crucial for *Regression* or *Classification* performance and, in particular, to achieve generalized models that are independent of:
>
> - illumination conditions
> - spectrometer sensitivity or exposure time
>
> See Table 3.1 for a comparison of the scaling methods of **TII Spectrometry**.

Scaling Methods

Min-Max Scaling

Min-Max scaling, also known as feature scaling or unity-based normalization, is a data preprocessing technique to transform numerical features to a specific, predefined range, usually $[0, 1]$.

For a single spectrum X_i, the transformation is:

$$X_{\text{MM},i} = \frac{X_i - \min(X_i)}{\max(X_i) - \min(X_i)}$$

Here:

- X_i is the original spectrum.
- $\min(X_i)$ and $\max(X_i)$ are the minimum and maximum absorbance/reflectance values within that single spectrum.

The primary goal of per-spectrum Min-Max scaling is to remove multiplicative scaling differences caused by factors like changes in path length, sample packing, or light source intensity that affect the magnitude of the spectrum.

- Baseline Anchor: This method forces the lowest point in the spectrum to 0 and the highest point to 1. This effectively corrects for differences in the dynamic range or overall spread of the signal intensity from one sample to the next.
- Contrast Preservation: It preserves the relative shape and proportionality of the spectral features, ensuring that the height ratios between peaks remain consistent.

Standard Normal Variate Scaling

SNV scaling is a per-spectrum operation, meaning it is applied independently to each individual spectral curve in a dataset. It is a two-step process that normalizes the spectrum based on its own mean and standard deviation. The Standard Normal Variate (SNV) scaling method is a common technique used in spectroscopy, particularly with Near-Infrared (NIR) data, to perform baseline correction and standardize spectral features. For a single spectrum X_i (a vector of measured values at different wavelengths), the transformation to the scaled spectrum $X_{\text{SNV},i}$ is given by:

$$X_{\text{SNV},i} = \frac{X_i - \bar{X}_i}{s_i}$$

Here:

- X_i is the original spectrum.
- $\bar{X}_i$ is the mean of all absorbance/reflectance values within that spectrum.
- s_i is the standard deviation of all absorbance/reflectance values within that spectrum.

This formula results in a new spectrum where the average intensity is centered near zero, and the variance (spread) is standardized to one.

SNV scaling effectively removes two major sources of variation that are not related to the sample's chemical composition:

1. Baseline Offset (Additive Effects): The subtraction of the mean ($\bar{X}_i$) corrects for constant vertical shifts in the spectrum caused by factors like changes in the sample path length or light scattering variations that affect the overall intensity level equally across all wavelengths.
2. Scaling Differences (Multiplicative Effects): Dividing by the standard deviation (s_i) corrects for variations in the slope or overall magnitude of the spectrum caused by differences in scattering properties, particle size, or instrument changes.

By removing these physical variations, SNV enhances the spectral features that are genuinely related to the chemical composition (the characteristic absorption peaks), making subsequent modeling more accurate and robust.

Table 3.1: Min-Max *vs.* SNV

Feature	Per-Spectrum Min-Max Scaling	Standard Normal Variate (SNV)
Centering Reference	**The absolute minimum value** of the spectrum.	**The mean value (**$\bar{X}_i$**)** of the entire spectrum.
Scaling Reference	**The range (**$\max - \min$**)** of the spectrum.	**The standard deviation (**s_i**)** of the spectrum.
Targeted Error	Primarily **Multiplicative scaling** (intensity differences).	Both **Additive baseline shifts** and **Multiplicative scaling**.
Effect on Peaks	Anchors the lowest point to 0 and stretches/compresses the peaks to fit between 0 and 1.	Centers the whole spectrum around 0, making the negative and positive peak areas equivalent in deviation.

See also

See the *Application Example Plastic Identification* (page 54) for a discussion of data preprocessing in the context of a pratical application.

3.4.3 Regression Analysis

As discussed above, *Regression* involves assigning numerical values to spectra.

TII Spectrometry offers two different methods to train *Regression* models (Table 3.2):

- manual training using linear regression[32]. This requires the selection of a relevant spectral feature, e.g. the area of a peak or the intensity ration of two peaks, from which a calibration curve is constructed. *Prediction* is performed using this calibration curve.
- semi-automated, machine-learning based regression based on Support Vector Regression (SVR)[33]. In contrast linear regression, which try to minimize the sum of squared errors, SVR tries to fit the best line or hyperplane while ensuring that most of the predicted data points are within a certain distance of that line. For non-linear relationships (which are common in spectral datasets), SVR uses the Kernel Trick (e.g., the Radial Basis Function or RBF kernel) to map the input features into a higher-dimensional space where a linear hyperplane can successfully model the non-linear relationship in the original space. This method is not only robust to noise and outliers but also can model complex, non-linear relationships between spectral features and continuous properties (like concentration or quality scores) using kernels. In contrast to linear regression, no feature selection by the user is required.

Table 3.2: Linear Regression *vs.* SVR

Feature	Linear Regression	Support Vector Regression (SVR)
Model Type	Parametric (Assumes a linear relationship).	Non-Parametric (Flexible, often uses kernels).
Objective Function	Minimizes the **Sum of Squared Errors (SSE)**, penalizing *all* errors equally.	Minimizes the errors that fall **outside** a defined margin (ϵ), ignoring small errors within the margin.
Error Treatment	**Sensitive** to all data points and outliers, especially those far from the line.	**Insensitive** to data points within the ϵ-tube; robust to noise and outliers.
Model Complexity	Simple, easy to interpret, fast to train.	More complex, computationally intensive, especially with kernel methods.
Non-Line	Cannot model non-linear relationships without manual feature engineering (e.g., polynomial terms).	Naturally handles **non-linear relationships** using the **Kernel Trick** (e.g., RBF kernel).
Key Points	Finds the line that best fits the **average** of the data.	Finds the line that best fits the **boundary** defined by the **Support Vectors**.
Application Suitability	Simple, well-behaved datasets where relationships are known to be linear.	High-dimensional, complex datasets (like spectral data) where non-linear modeling and noise robustness are required.

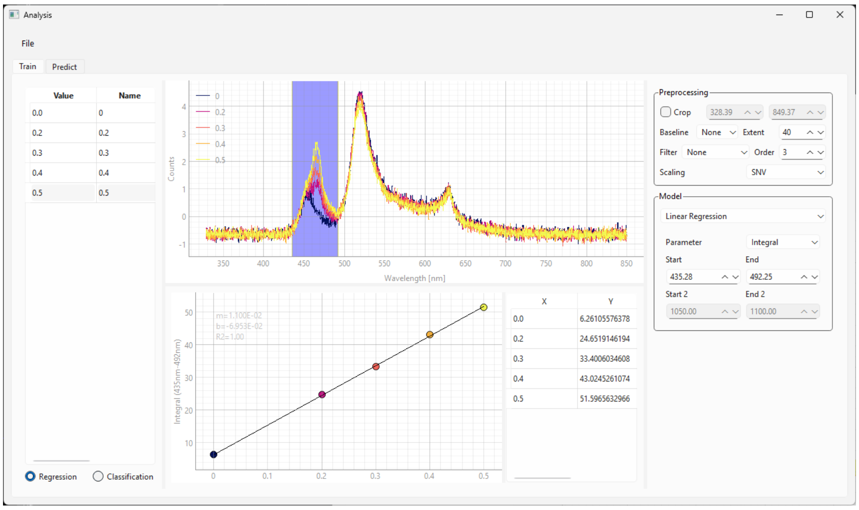
Training

Linear Regression

The *Train* view (*Analysis* ‣ *Modeling* ‣ *Train/Predict*, Figure 3.12) contains the following user interface elements:

- the spectra sidebar on the left, which contains the spectra used for training as well as their labels
- the spectrum view, which contains the spectra after pre-processing
- the parameter sidebar on the right, which controls pre-processing and training settings
- the result view (center bottom), which contains the calibration curve and the predicted numerical value for each training spectrum.

[32] https://en.wikipedia.org/wiki/Linear_regression
[33] https://en.wikipedia.org/wiki/Support_vector_machine



Value	Name
0.0	0
0.2	0.2
0.3	0.3
0.4	0.4
0.5	0.5

X	Y
0.0	6.26105576378
0.2	24.6519146194
0.3	33.4006034608
0.4	43.0245261074
0.5	51.5965632966

☐ Crop 328.39 849.37

Baseline None Extent 40

Filter None Order 3

Scaling SNV

Linear Regression

Parameter Integral

Start 435.28 End 492.25

Start 2 1050.00 End 2 1100.00

● Regression

Fig. 3.12: The *Training* view of the *Modeling Window*

To train a *Regression Model*:

1. display the *Modeling* window using *Analysis* ‣ *Modeling* ‣ *Train/Predict* (Figure 3.12).
2. select the *Train* tab (the *Train* tab is shown in Figure 3.12).
3. select *Regression* from the radio button set below the left sidebar
4. load a dataset. This can be done by:
   - dragging spectra from the *spectra side bar* (page 6) into the left sidebar of the *Modeling* window
   - dragging a saved file (in `.hdf5` format) onto the left sidebar

   The spectra contained in the file will now appear in the sidebar and the spectrum view
5. apply numerical labels to each spectrum. This can be done by:
   - `double-clicking` on the cell in the *Value* column
   - entering a numerical value, e.g. a concentration

Hint

Since labeling can be tedious, labeled datasets can be saved using *File* ‣ *Save Dataset*.

6. select appropriate *pre-processing* (page 35) parameters.

Tip

The spectra in the spectra view will reflect the current preprocessing settings.

For the data in Figure 3.12 in we have :

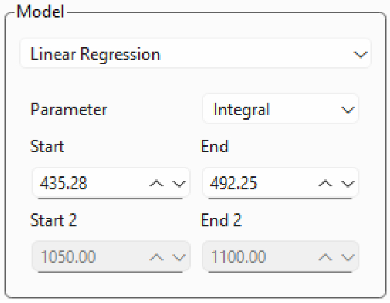
- cropped the spectral range between 400 and 800 nm
- applied SNV *scaling* (page 36)

Important

Scaling is generally recommended for satisfactory model performance. Please see the discussion in Section 3.4.2 for details.

See also

For this example, we are training a *linear regression model* (page 37), which requires manual feature selection. For training a *Support Vector Regression* (page 38) model, jump forward to Section 3.4.3.



Model

Linear Regression

Parameter: Integral

Start: 435.28

End: 492.25

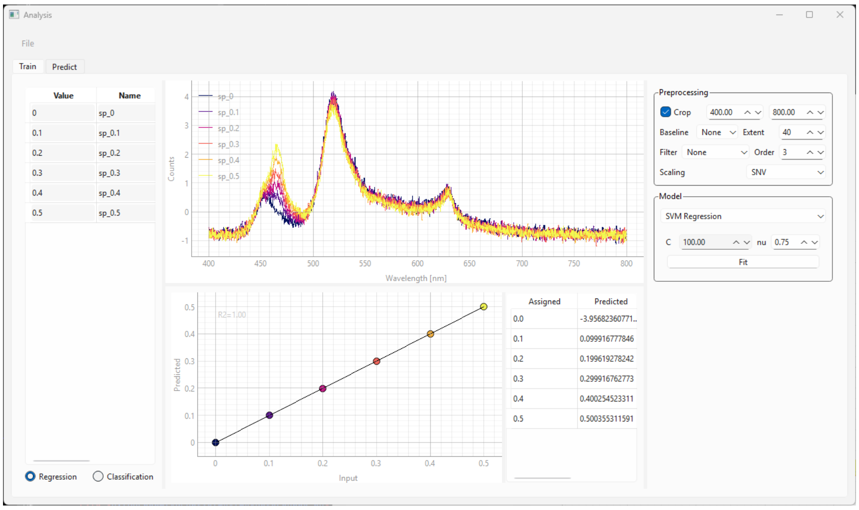
Start 2: 1050.00

End 2: 1100.00

Fig. 3.13: Linear Regression Settings

7. Figure 3.13 displays the settings for a linear regression analysis.
   - *Parameter*: Allows the selection of a spectral parameter, e.g. an integral, peak width, or peak area ratio. Please see Section 3.1 for available parameters and their definition.
   - *Start* and *End* determine the spectral range from which the parameter is computed. This parameter can also be adjusted by dragging and resizing the region selector in the spectrum view.
   - for peak ratios, the *Start 2* and *End 2* settings will become available
8. The *Calibration Curve* (bottom of Figure 3.12) will reflect the settings. Adjust settings until the linear trendline matches the data.
   - the table adjacent to the calibration curve shows the *X* and *Y* values of the curve
   - slope, y-intercept, and R^2 value are displayed in the calibration curve graph
9. If you are satisfied with the model, switch to the *Predict* tab (Section 3.4.3).
10. (optional) Save the model to disk using *File* ‣ *Save Model*.

Support Vector Regression



Value	Name
0	sp_0
0.1	sp_0.1
0.2	sp_0.2
0.3	sp_0.3
0.4	sp_0.4
0.5	sp_0.5

Preprocessing
☑ Crop 400.00 800.00
Baseline None Extent 40
Filter None Order 3
Scaling SNV

Model
SVM Regression
C 100.00 nu 0.75

Assigned	Predicted
0.0	-3.95682360771..
0.1	0.099916777846
0.2	0.199619278242
0.3	0.299916762773
0.4	0.400254523311
0.5	0.500355311591

Fig. 3.14: The *Training* view of the *Modeling Window* (SVR)

Loading data, assigning labels, and preprocessing are identical between linear regression and SVR models (steps 1-6 in Section 3.4.3).

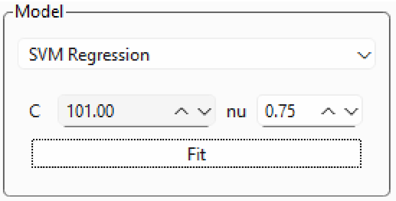

Model
SVM Regression
C 101.00 nu 0.75

Fig. 3.15: SVR Settings

Figure 3.15 shows a close-up of the *SVR* settings box, which has two parameters:

C

The parameter C controls the trade-off between model complexity and the degree of tolerance for training errors.

- A small C means a weak penalty. The model allows more points to violate the margin, resulting in a smoother, simpler hyperplane (higher bias, lower variance). This is often desired if the data is very noisy.
- A large C means a strong penalty. The model tries hard to include almost all training points within the margin, resulting in a more complex, wiggly hyperplane (lower bias, higher variance). This can lead to overfitting if the data is noisy.

ν (Nu)

ν places an upper bound on the fraction of training errors (outliers that fall outside the margin) and a lower bound on the fraction of Support Vectors relative to the total number of training points. ν must be between 0 and 1. ν implicitly determines the value of ϵ, which is used in some SVM implementations.

- A small ν (e.g., 0.1): Allows for a tighter margin and fewer outliers. This corresponds to the model being more restrictive, similar to a high ϵ
- A large ν (e.g., 0.9): Allows for a wider margin and more potential outliers/Support Vectors.

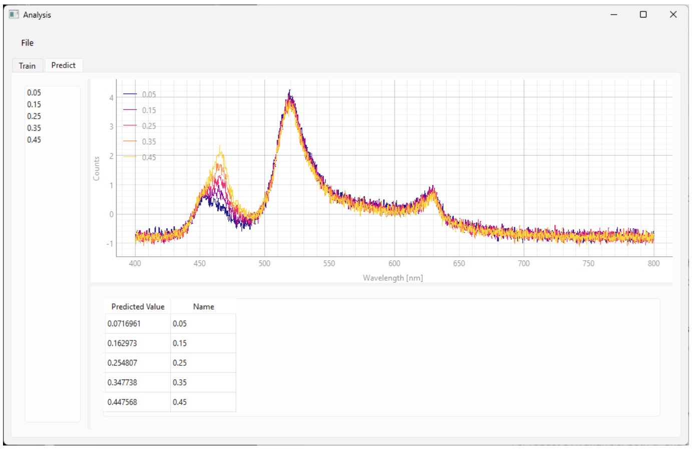
Fit

Click the *Fit* button to train the model. This will update the *result graph* and *result table*.

The *SVR* algorithm automatically extracts the relevant spectral features for regression from the dataset. The resulting curve is shown in at the bottom of the Train *window* (page 41). The curve displays the assigned (*Input*) vs *Predicted* numerical value - ideally this should be a straight line with slope 1 and datapoints should coincide with the black line. The table on the right side of the graph displays the numerical values of the assigned labels.

Prediction

To use a model, select the *Predict* tab (Figure 3.16).



Predicted Value	Name
0.0716961	0.05
0.162973	0.15
0.254807	0.25
0.347738	0.35
0.447568	0.45

Fig. 3.16: The *Predict* screen (SVR)

The *Predict* tab will contain the last trained model from the *Train* tab. Alternatively, you can load a model from disk using *File* ‣ *Load Model*.

Tip

You can switch back and forth between the *Train* and *Predict* screens to optimize model training using cross-validation.

To use a model:

1. load data by dragging a `.hdf5` file onto the left sidebar. This will:
    - open the spectra
    - apply the processing selected in the model
    - perform the regression analysis
2. the results can be found in the table at the bottom. It contains:
    - the predicted numerical value
    - the name of the spectrum

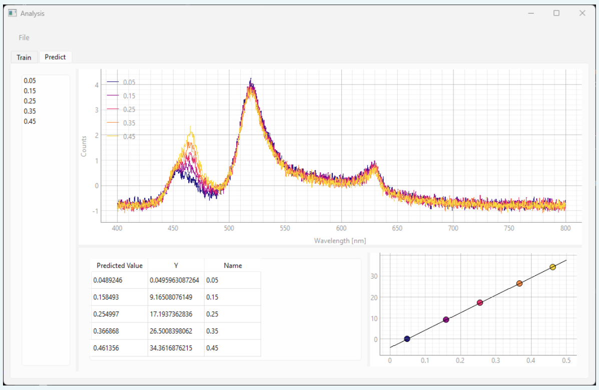
In the example in Figure 3.16, the spectra were recorded at known concentrations so this dataset can be used for validation. The concentrations in the validation dataset are different from the concentrations employed during training. The *Name* column contains the (known) correct value of the predicted parameter. It can be seen that the agreement between predicted and correct validation value is very good, which indicates that we have successfully trained the model.

Note

For *linear regression models* (page 38),

- the result table in the *Predict* screen also contains the extracted spectral parameter (e.g. integrated peak are) in the *Y* column
- the *Predict* screen displays the calibration curve and the position of the of the samples on the curve.

See Figure 3.17 for an example.



Predicted Value	Y	Name
0.0489246	0.0495963087264	0.05
0.158493	9.16508076149	0.15
0.254997	17.1937362836	0.25
0.366868	26.5008398062	0.35
0.461356	34.3616876215	0.45

Fig. 3.17: The *Predict* screen (Linear Regression)

3.4.4 Classification Analysis

For *Classification*, **TII Spectrometry** offers Support Vector Machine (SVM)[34] Classification. Analogous to *Support Vector Regression (SVR)* (page 38), the goal of SVM classification is to find the hyperplane that has the largest margin between the nearest training data points of any class.

See also

Many of the remarks on *Support Vector Regression* (page 38) also apply to SVM classification.

Training

Training a *Classification* model generally mirrors the steps laid out in Section 3.4.3:

1. display the *Modeling* window using *Analysis* ‣ *Modeling* ‣ *Train/Predict* (Figure 3.18).
2. select the *Train* tab (the *Train* tab is shown in Figure 3.18).
3. select *Classification* from the radio button set below the left sidebar
4. load a dataset.
5. apply labels to the dataset. Labels can any text.

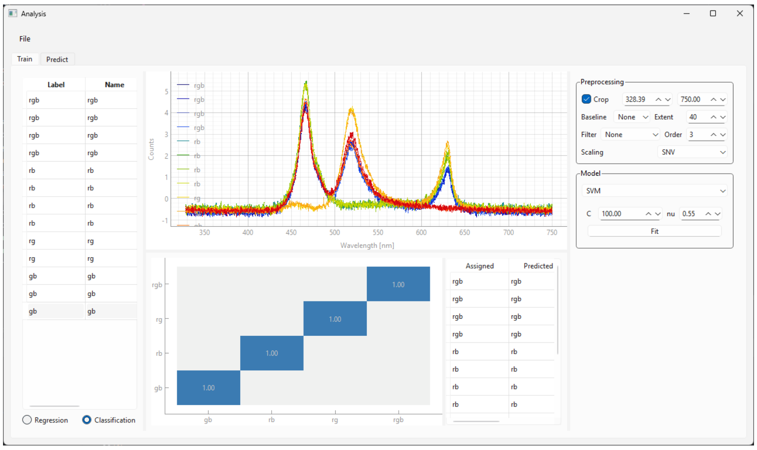
Tip

Labeled datasets can be saved to disk

6. adjust the *SVM* hyperparameters C and ν (Section 3.4.3) and click *Fit* to train the model.
7. the *result view* at the bottom shows the confusion matrix[35], which plots the predicted vs. assigned label. Ideally, all values fall on the diagonal.
8. if you are satisfied with the model, switch to the Predict (page 44) tab.

[34] https://en.wikipedia.org/wiki/Support_vector_machine

[35] https://en.wikipedia.org/wiki/Confusion_matrix



Label	Name
rgb	rgb
rgb	rgb
rgb	rgb
rgb	rgb
rb	rb
rb	rb
rb	rb
rb	rb
rg	rg
rg	rg
gb	gb
gb	gb
gb	gb

Preprocessing

☑ Crop 328.39 750.00

Baseline None Extent 40

Filter None Order 3

Scaling SNV

Model

SVM

C 100.00 nu 0.55

Fit

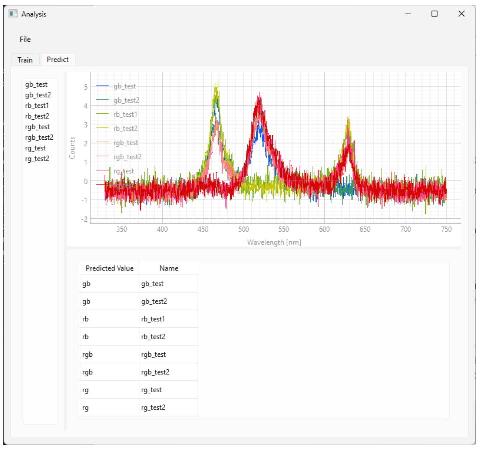
Assigned	Predicted
rgb	rgb
rgb	rgb
rgb	rgb
rgb	rgb
rb	rb
rb	rb
rb	rb
rb	rb

Fig. 3.18: Training a *Classification* model.

Prediction

Using a trained *classification* model for prediction mirrors the use of regression *models* (page 42). Simply:

1. Load a dataset by dropping a `.hdf5` file onto the left sidebar.
2. The classification result will be shown in the table at the bottom (Figure 3.19)



gb_test
gb_test2
rb_test1
rb_test2
rgb_test
rgb_test2
rg_test
rg_test2

Predicted Value	Name
gb	gb_test
gb	gb_test2
rb	rb_test1
rb	rb_test2
rgb	rgb_test
rgb	rgb_test2
rg	rg_test
rg	rg_test2

Fig. 3.19: Using a *Classification* model.

For the dataset in Figure 3.19, the first part of the name of the spectra used for prediction contains the correct label. It can be seen that the agreement of the predicted value with the correct label is excellent.

3.4.5 Monitoring

You can use trained models (both *Classification* and *Regression* models) in **TII Spectrometry** for real-time monitoring, for example:

- to monitor a concentration using a *Regression* model
- to identify different substances

This functionality can be accessed using *Analysis* ‣ *Modeling* ‣ *Monitor* to show the *Monitoring* screen (Figure 3.20). Here,

- you can load a model using the *Load* button

When using the spectrometer in *single or continuous acquisition mode* (page 4), the prediction result of the selected model for the currently acquired spectrum will be shown in the top right.

> **Important**
>
> The prediction results are only displayed but not saved to disk. To record prediction results, use a *time-lapse acquisition* (page 23).

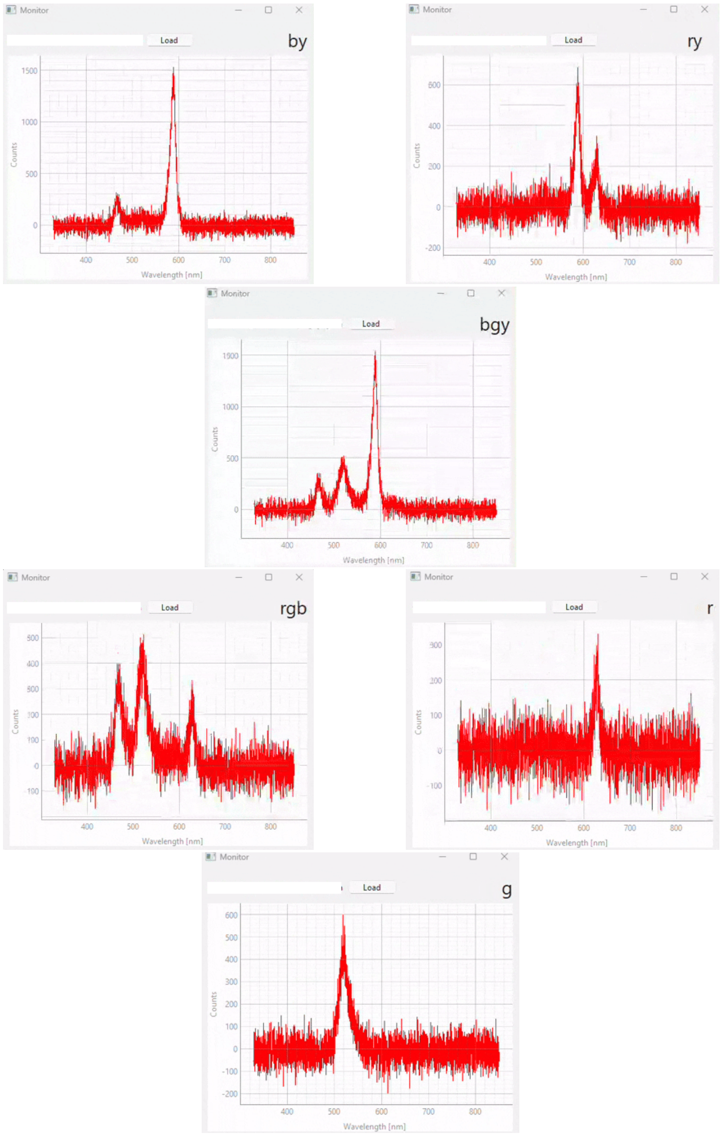
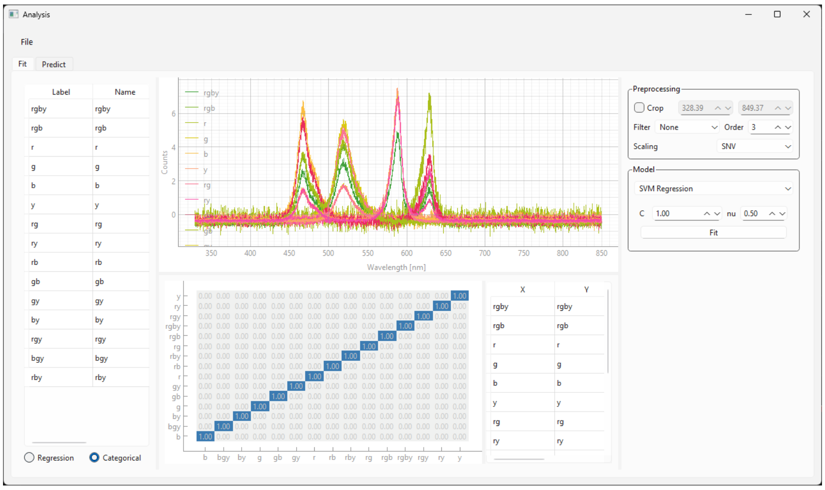


Fig. 3.20: Real-time monitoring (snapshots)

Figure 3.20 displays snapshots of the prediction result at different points in time. The dataset / model used in this experiment (which contains many different sample classes) is displayed in Figure 3.21. It is important to note that:

- the signal-to-noise ratio of the test spectra (during monitoring) is a lot lower than the SNR of the spectra used for training. Due to appropriate scaling and the relatively noise-tolerant SVM model, this has no detrimental effect during the prediction stage.
- prediction fidelity is excellent - there are no misclassifications



Label	Name
rgby	rgby
rgb	rgb
r	r
g	g
b	b
y	y
rg	rg
ry	ry
rb	rb
gb	gb
gy	gy
by	by
rgy	rgy
bgy	bgy
rby	rby

○ Regression ● Categorical

Preprocessing

☐ Crop 328.39 849.37

Filter None Order 3

Scaling SNV

Model

SVM Regression

C 1.00 nu 0.50

	b	bgy	by	g	gb	gy	r	rb	rby	rg	rgb	rgby	rgy	ry	y
y	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
ry	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
rgy	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
rgby	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
rgb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
rg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
rby	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00
rb	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
r	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
gy	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
gb	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
g	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
by	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
bgy	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
b	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

X	Y
rgby	rgby
rgb	rgb
r	r
g	g
b	b
y	y
rg	rg
ry	ry

Fig. 3.21: The *Classification* model used for the monitoring experiment.

CHAPTER

FOUR

APPLICATION EXAMPLES

4.1 The Solar Spectrum

Spectral calibration is also relevant when *multiple spectrometers* (page 17) with overlapping or adjacent spectral ranges are used to record the spectrum of the same light source (see scheme in Figure 4.1). Figure 4.3 displays the spectrum of the sun using two spectrometers that cover the visible and near-infrared range of the solar spectrum.

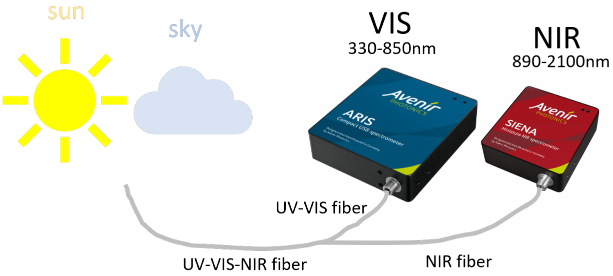


Fig. 4.1: Measuring the spectrum of the sun using two spectrometers

Both spectrometers (page 12) (and their input fibers) were calibrated using the same reference light source according to the procedure outlined in Section 2.1.6 (*Intensity Calibration* (page 9)).

1. The spectrum of a reference light source (incandescent lamp with a color temperature of 2600 K) was acquired using both spectrometers (Figure 4.2 left). The decrease in sensitivity at NIR wavelengths of the VIS spectrometer (700-800 nm) is clearly visible. It is obvious that the spectrum doesn't match the expected shape of a tungsten lamp at all.

2. The reference intensity curve was calculated using the known color temperature of the reference light source in the spectral range between 200-3000 nm using *Planck's Law*[36] (4.1).

$$I = \frac{2hc^2}{\lambda^5} \frac{1}{\exp(\frac{hc}{\lambda k_B T}) - 1} \tag{4.1}$$

   Here, h is *Planck's constant*, c is the speed of light, $\mathrm{k_B}$ is Boltzmann's constant, T is the absolute temperature of the black body emitter, and λ is the wavelength.

3. The calibration data was applied to the two spectrometers. This results in a intensity-corrected spectrum of the reference light source (Figure 4.2 right).

[36] https://en.wikipedia.org/wiki/Planck%27s_law

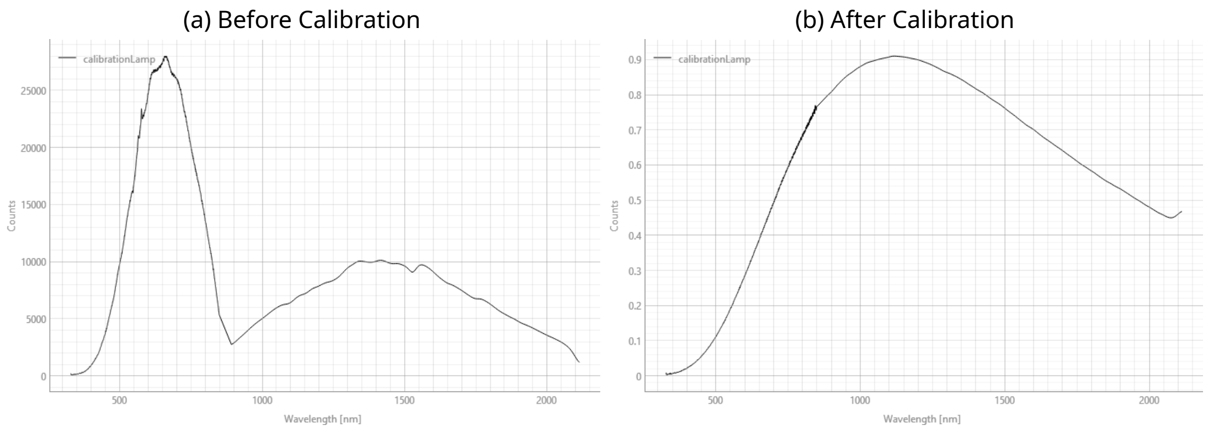

(a) Before Calibration
(b) After Calibration

Fig. 4.2: Calibrating two spectrometers

After intensity calibration of both spectrometers, the recorded spectrum of the sun (Figure 4.1) matches that of a black body emitter with a color temperature > 5000 K (deviations are due to atmospheric scattering, which increase when the input fiber is pointed away from the sun). Fraunhofer lines are visible in the spectrum. Fraunhofer lines are a set of dark spectral absorption lines observed in the continuous spectrum of the Sun and other stars that reveal the chemical composition of stellar atmospheres. Note that some dark lines, like the A and B bands, are Telluric lines, meaning they are caused by absorption by molecules (primarily oxygen (O_2) and water vapor (H_2O)) in the Earth's own atmosphere, rather than the Sun's.

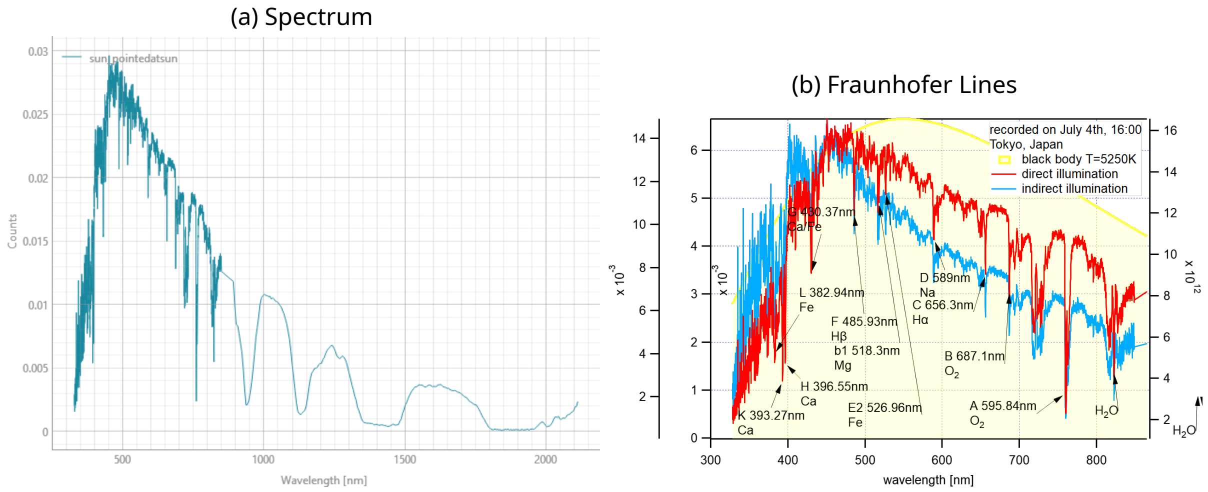

(a) Spectrum
(b) Fraunhofer Lines

Fig. 4.3: The spectrum of the sun

See also

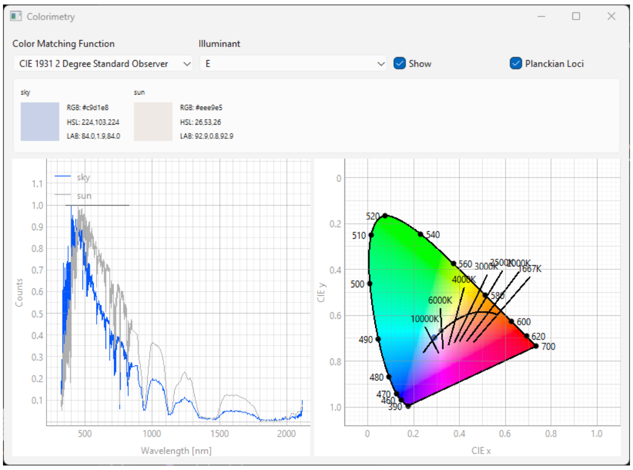
The solar spectrum will be further analyzed in the *Application Examples* *Radiometric Analyis of Light Sources* (page 51) & *Colorimetric Analysis of the Spectrum of the Sun* (page 49).

4.2 Colorimetry of Light Sources & Color Charts

This section provides practical tips and tricks as well as some application examples on *colorimetric analysis*. See Section 3.2 for background and a description of the parameters and user interface.

4.2.1 Colorimetric Analysis of the Spectrum of the Sun

We can re-use the spectra obtained in Section 4.1 (*The Solar Spectrum* (page 47)) for colorimetric analysis. Here, we are using the illuminant *E* (page 28), which is a flat curve (black trace in Figure 4.4), since spectra were obtained from an emissive source. Only the visible region of the spectrum is used for analysis and hence the majority of the spectrum, which falls into the mid-IR range, is ignored.



Colorimetry

Color Matching Function: CIE 1931 2 Degree Standard Observer

Illuminant: E

☑ Show

☑ Planckian Loci

sky
RGB: #c9d1e8
HSL: 224,103,224
LAB: 84.0,1.9,84.0

sun
RGB: #eee9e5
HSL: 26,53,26
LAB: 92.9,0.8,92.9

Fig. 4.4: Colorimetric Analysis - Spectrum of the Sun

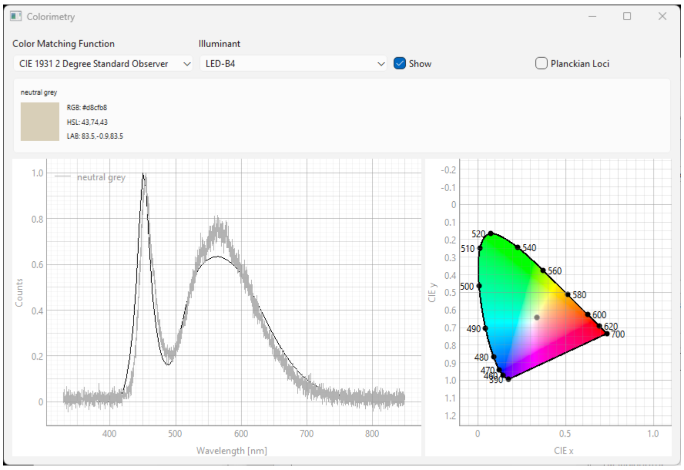
When the spectrometer input fiber pointed directly at the sun (gray trace in the left panel of Figure 4.4), the calculated color is a bright, slightly yellow-white, as expected. When light is collected indirectly by pointing the input fiber away from the sun, the color shifts to a cool, bluish-white (blue trace in the right panel of Figure 4.4), matching the expected blue color of the sky on a clear day. The position in the *chromaticity diagram* (page 27) of both spectra coincides with the line of a black body emitter (*Planckian Loci* (page 28), black line in the right panel of Figure 4.4). This means both light sources (the sun itself and the scattered light from the sky) match the ideal color of a thermal radiator. The spectrum of the sun (circle with gray outline) corresponds to a color temperature of approximately 6000 K, which is a value typical for direct sunlight filtered by the atmosphere. On the other hand, the spectrum of the sky (circle with blue outline) suggests a color temperature of almost 10000 K. This indicates that there is a significant amount of atmospheric scattering (Rayleigh scattering $I_{s,\mathrm{Rayleigh}} \propto 1/\lambda^4$) caused by the relatively low position of the sun in the sky due to latitude and time of day. Since light at short wavelengths (blue light) is more effectively scattered by air molecules than red light, atmospheric scattering will blue-shift the spectrum. This matches the observations in Figure 4.3 that were obtained by comparing the raw spectra with the expected curve of a black body emitter with the temperature of the sun (5800 K).

4.2.2 Reflective Colorimetric Analysis

In this section, spectra were obtained using a small, handheld spectrometer using light reflected from a printed color sample. The sample was illuminated by LED lamps (room lighting of an office environment) and spectra were recorded by placing the entrance pupil of the spectrometer close to the color sample at a shallow angle to the surface normal. The displayed spectra are the raw data from the spectrometer; no *dark / background subtraction* (page 7) or *intensity correction* (page 9) was performed.

Tip

For colorimetric analysis, the spectrum is analyzed in the range between 400-700 nm. If the sensitivity curve of the spectrometer is not reasonably flat in this spectral range, performing a *intensity calibration* (page 9) is recommended for best results.



Color Matching Function: CIE 1931 2 Degree Standard Observer

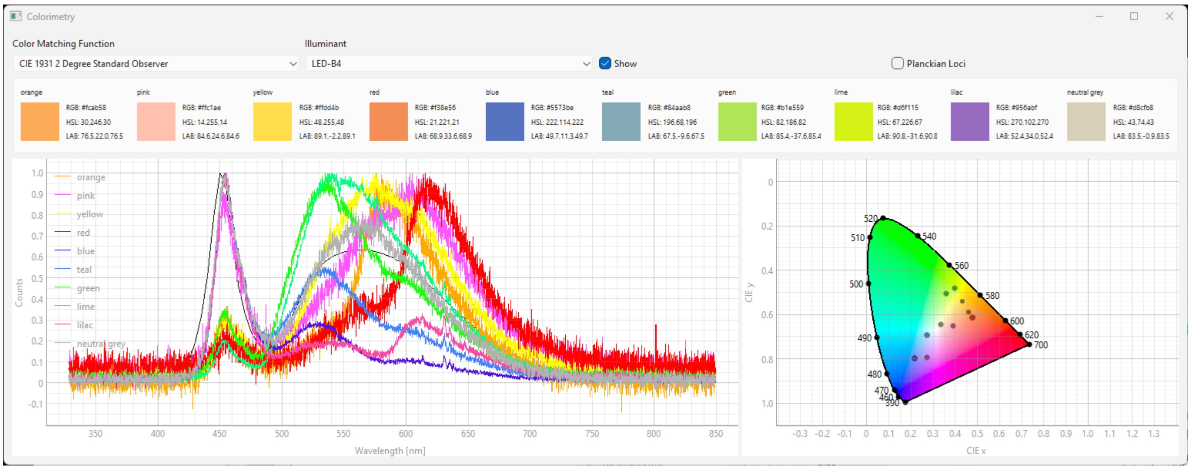
Illuminant: LED-B4 ☑ Show

☐ Planckian Loci

neutral grey
RGB: #d8cfb8
HSL: 43,74,43
LAB: 83.5,-0.9,83.5

Fig. 4.5: Colorimetric Analysis - Illuminant

Figure 4.5 shows the spectrum reflected of an office desk with a bright white color. The black line represents the *LED-B4 illuminant* (page 28), a bright white LED light source with a color temperature of 5100 K, which is typical for office settings. The two spectra roughly match, indicating that this illuminant is a good choice to represent the light source used in this experiment. The calculated color is a slightly yellowish gray, which reasonably matches the visual perception of the desk's color.



Color Matching Function: CIE 1931 2 Degree Standard Observer

Illuminant: LED-B4 ☑ Show

☐ Planckian Loci

	RGB	HSL	LAB
orange	#fcab58	30,246,30	76.5,22.0,76.5
pink	#ffc1ae	14,255,14	84.6,24.6,84.6
yellow	#ffdd4b	48,255,48	89.1,-2.2,89.1
red	#f38e56	21,221,21	68.9,33.6,68.9
blue	#5573be	222,114,222	49.7,11.3,49.7
teal	#84aab8	196,68,196	67.5,-9.6,67.5
green	#b1e559	82,186,82	85.4,-37.6,85.4
lime	#d6f115	67,226,67	90.8,-31.6,90.8
lilac	#956abf	270,102,270	52.4,34.0,52.4
neutral grey	#d8cfb8	43,74,43	83.5,-0.9,83.5

Fig. 4.6: Colorimetric Analysis

Figure 4.6 displays spectra obtained from different color samples (with the names taken from the color sample's description) in the left pane. All spectra have been normalized, which is automatically done prior to analysis. Significant spectral differences even for perceptualy 'close' colors (e.g. green and lime) can be observed. Using the correct illuminant, the calculated color and visually perceived color match quite well over a wide range of different colors. Color fidelity could be further improved by:

- standardized illumination
- more repeatable spectrum collection, i.e. avoiding specular reflections and shadowing, and maintaining a constant reflection angle.
- intensity calibration, though the effect will likely be very minor
- an improved signal-to-noise ratio for some of the spectra

4.3 Radiometric Analyis of Light Sources

This section describes the practical application of Radiometry (page 29) in the analysis of the emitted power and color fidelity of different light sources.

The investigated light sources are:

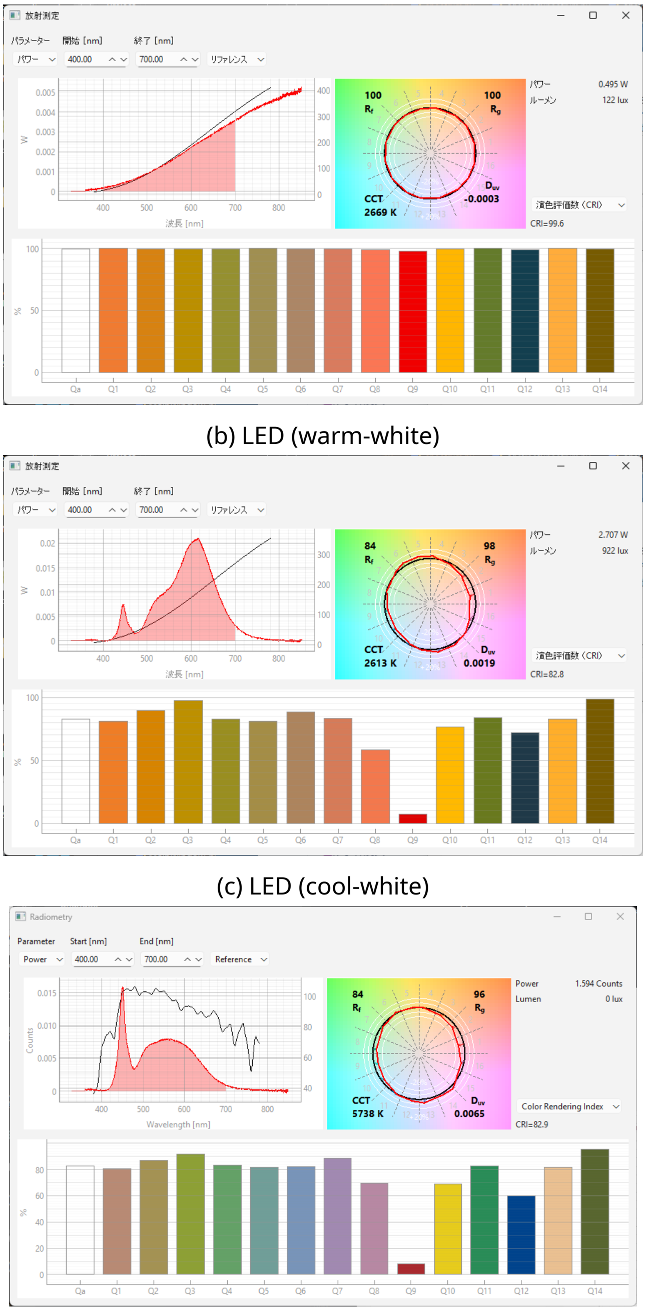
1. an incandescent lamp with known output power that serves as the calibration source.
2. a warm-white LED lamp (Toshiba LDA8L-G[37]) with a nominal *color temperature* (page 32) of 2700 K and an R_α (page 32) of 80
3. a cool-white LED (Panasonic LDA4DGK4[38]) with a nominal color temperature of 6500 K and an R_α of 84.

LED light sources were mounted in an integrating sphere. The spectrometer was calibrated using the procedure outlined in Section 2.1.6 using the incandescent calibration lamp, which is integrated into the integrating sphere. The spectrometer's exposure time was adjusted before each light source change and after the calibration to avoid saturating the detector while maintaining a acceptable signal-to-noise ratio. The results are shown in Figure 4.7 (the result for the cool-white LED is shown without power calibration).

[37] https://saturn.tlt.co.jp/pdocs/s/LDA8LG60W

[38] https://www2.panasonic.biz/jp/catalog/lighting/products/detail/shouhin.php?at=keyword&amp;ct=zentai&amp;id=S00327316

(a) Incandescent



放射測定

パラメーター: パワー　開始 [nm]: 400.00　終了 [nm]: 700.00　リファレンス

パワー 0.495 W
ルーメン 122 lux
演色評価数 (CRI)
CRI=99.6

R_f 100　R_g 100　CCT 2669 K　D_{uv} -0.0003

(b) LED (warm-white)

放射測定

パラメーター: パワー　開始 [nm]: 400.00　終了 [nm]: 700.00　リファレンス

パワー 2.707 W
ルーメン 922 lux
演色評価数 (CRI)
CRI=82.8

R_f 84　R_g 98　CCT 2613 K　D_{uv} 0.0019

(c) LED (cool-white)

Radiometry

Parameter: Power　Start [nm]: 400.00　End [nm]: 700.00　Reference

Power 1.594 Counts
Lumen 0 lux
Color Rendering Index
CRI=82.9

R_f 84　R_g 96　CCT 5738 K　D_{uv} 0.0065

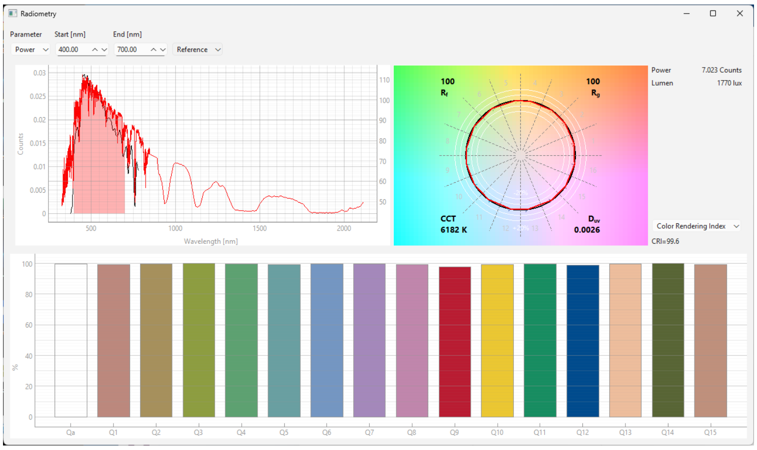
Fig. 4.7: Radiometric analysis of various light sources

4.3.1 Results - Color Quality

- the *perceived brightness* (page 30) of the warm-white LED (about 900 lm) slightly exceeds the nominal value. This value gradually decreases as the LED heats up. It is likely that the manufacturer’s specifications are minimum limits.
- the incandescent lamp has a *color rendering index (CRI)* (page 32) (R_a) close to 100, as expected from the definition of the CRI. The (calculated) reference curve closely matches the spectrum
- the warm-white LED has a CRI (R_a) of 83, slightly exceeding specifications
- the cool-white LED has a CRI (R_a) of 83, slightly below specification
- the warm-white LED and the incandescent lamp have a similar *color temperature* (page 32) and hence render the test color samples very similarly. The biggest exception is color #9

(deep red), which is poorly rendered by the LED

- the cool-white LED shows a similar deficiency for color #9, but (as expected), the other colors are rendered more realistically due to its higher CCT. This is particularly apparent for color #13, which represents a typical skin tone.
- the color temperature of the cool-white LED (5700 K) is quite a bit lower than the specification. It is not clear why this is the case, but it might be due to aging of the blue LED component.
- the D_{uv} *value* (page 32) for the incandescent lamp is close to 0. For the LEDs, the D_{uv} is slightly positive, indicating a subtle greenish tint characteristic of white-pumped LEDs
- for the warm-white LED and the incandescent lamp, a (calculated) black-body emitter curve is used as *reference* (page 30), while for the cool-white LED, the CIE Daylight data is used



Radiometry

Parameter: Power; Start [nm]: 400.00; End [nm]: 700.00; Reference

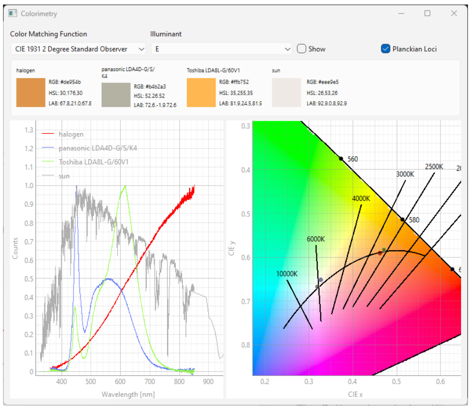
Power 7.023 Counts
Lumen 1770 lux

Color Rendering Index
CRI=99.6

Fig. 4.8: Radiometric analysis of the spectrum of the sun

We can compare this with the spectrum of the sun from Section 4.1, which is shown without power calibration (Figure 4.8). Being a black-body emitter, the spectrum of the sun also has a CRI of 100 and a color temperature > 6000 K. The dips in the CIE Daylight reference spectrum nicely coincide with the measured Fraunhofer lines (see also Figure 4.3). Comparing the sun with the cool-white LED, which has a similar *color temperature* (page 32), shows that sunlight renders all test colors with equally high fidelity, whereas the LED fails in particular at highly-saturated red (color #9). The D_{uv} is, maybe surprisingly, quite high and comparable to the D_{uv} of the warm-white LED in magnitude. This is likely a result of atmospheric scattering blue-shifting the solar spectrum.

4.3.2 Color Temperature & Planckian Loci



Colorimetry

Color Matching Function: CIE 1931 2 Degree Standard Observer
Illuminant: E
☐ Show
☑ Planckian Loci

halogen: RGB: #de954b, HSL: 30,176,30, LAB: 67.8,21.0,67.8
panasonic LDA4D-G/S/K4: RGB: #b4b2a3, HSL: 52.26.52, LAB: 72.6.-1.9.72.6
Toshiba LDA8L-G/60V1: RGB: #ffb752, HSL: 35,255,35, LAB: 81.9,24.5,81.9
sun: RGB: #eee9e5, HSL: 26,53,26, LAB: 92.9,0.8,92.9

Fig. 4.9: Comparison of LED and incandescent light sources and their color temperature.

Figure 4.9 shows a comparison of all four light sources (warm-white and cool-white LED, incandescent lamp, sun) in the *colorimetry view* (page 26). The positions of all four light sources (more or less) fall on the curve of *Planckian Loci* (page 28), which indicates that they all match the spectral characteristics of a black body emitter, albeit at different color temperatures. For the actual black body emitters (the sun and the incandescent lamp, red and grey outlined circles), the coincidence is noticeably better compared to the LEDs (blue and green outlined circles). The LEDs, being solid-state emitters, have discontinuous (peaked) spectral power distributions, which will always result in a measurable offset from the continuous Planckian Locus, even if their CCT is close. The differences in color temperature and quality of a neutral test target is illustrated by the calculated colors - sunlight clearly has the whitest, most neutral rendition whereas the lower color temperature sources cause a significant warmer tint.

4.4 Plastic Identification

4.4.1 Mid-Infrared Spectroscopy

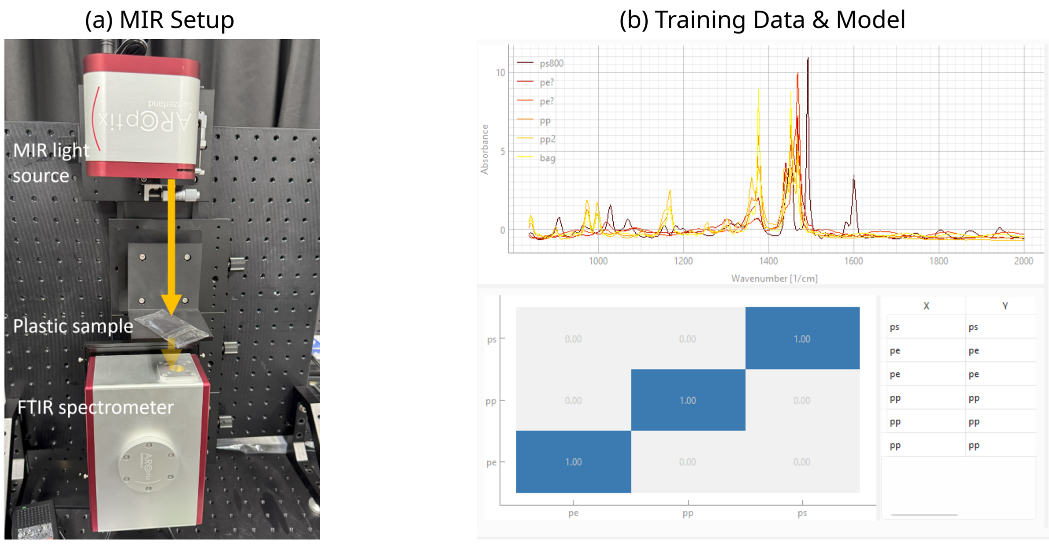
Mid-Infrared (Mid-IR) spectroscopy, operating in the 4000 cm^{-1} to 400 cm^{-1} wavenumber range, is the gold standard for identifying and classifying different types of plastics. When mid-IR light hits a plastic sample, the chemical bonds within the polymer chains (like C-H, C=O, and C-C bonds) absorb energy at specific, characteristic frequencies. This absorbed energy causes the bonds to vibrate (stretch, bend, rock, etc.). Since every type of plastic (e.g., Polyethylene, Polypropylene, PET) has a unique combination and arrangement of these chemical bonds, it produces a distinct pattern of absorption peaks. This pattern is called the infrared absorption spectrum or molecular fingerprint.

The measurement setup for plastic identification is shown in Figure 4.10 (left panel).

- A mid-IR light source (top) illuminates the sample. Transmitted IR light is directly collected by an *FTIR spectrometer* (page 13).
- Absorbance spectra are collected in the transmission geometry, meaning that thin plastic films are placed directly in the beam.
- Absorbance was calculated using the procedure outlined in Section 2.1.4.
- single FTIR scans without averaging were acquired, resulting in a cycle time of around 200 ms.
- three household plastic samples were used: polystyrene (PS), polyethylene (PE), and polypropylene (PP)
- the resulting *SVM Classification* (page 43) model is displayed in Figure 4.10 (right panel).
  - the spectral region of interest was cropped to the fingerprint region between 800 cm^{-1} and 2000 cm^{-1}.

    > **Note**
    >
    > Cropping was primarily done to remove the highly absorbing C-H stretch region around 2900 cm^{-1}, where very little light reaches the detector. This results in very high and fluctuating absorbance, which is detrimental to proper *data scaling* (page 36). It is important to note that the fingerprint region contains the relevant information for differentiating the plastic samples. In contrast, the high-energy C-H stretch region is common to all organic polymers and hence of little use for classification.

  - the data was scaled using *SNV scaling* (page 36) - the data shown in Figure 4.10 reflects this
  - the *confusion matrix* (page 43) in Figure 4.10 indicates that a classifier that can distinguish the three different types of plastic has been trained successfully.



(a) MIR Setup

(b) Training Data & Model

X	Y
ps	ps
pe	pe
pe	pe
pp	pp
pp	pp
pp	pp

Fig. 4.10: Plastic Classification by Mid-IR Spectroscopy

Figure 4.11 displays snapshots of real-time plastic identification using the Monitoring (page 44) view of **TII Spectrometry**. Here, plastic samples were inserted into the mid-IR light beam while continuously acquiring spectra. The samples were different from the training samples but of known composition in order to verify classifier accuracy.

- accuracy was generally excellent provided sufficient light could pass through the sample - the transmission setup will fail for thick samples
- *SNV scaling* (page 36) does a good job of standardizing the overall intensity and removing baseline curvature. Hence, the SVM model is forced to focus exclusively on the shape and position of the characteristic peaks—the true chemical information. This results in a model that can - within reason - classify samples of different thickness (and hence difference absorbance) using transmission mid-IR spectroscopy.
- spectral differences between the three types of plastic are very obvious in the mid-IR - it is hence no surprise that the classifier performs well
- no blank spectra were included during training. This is the reason for the misclassification of the blank spectrum in Figure 4.11 as *PE*
- the model could easily be extended to incorporate more sample classes

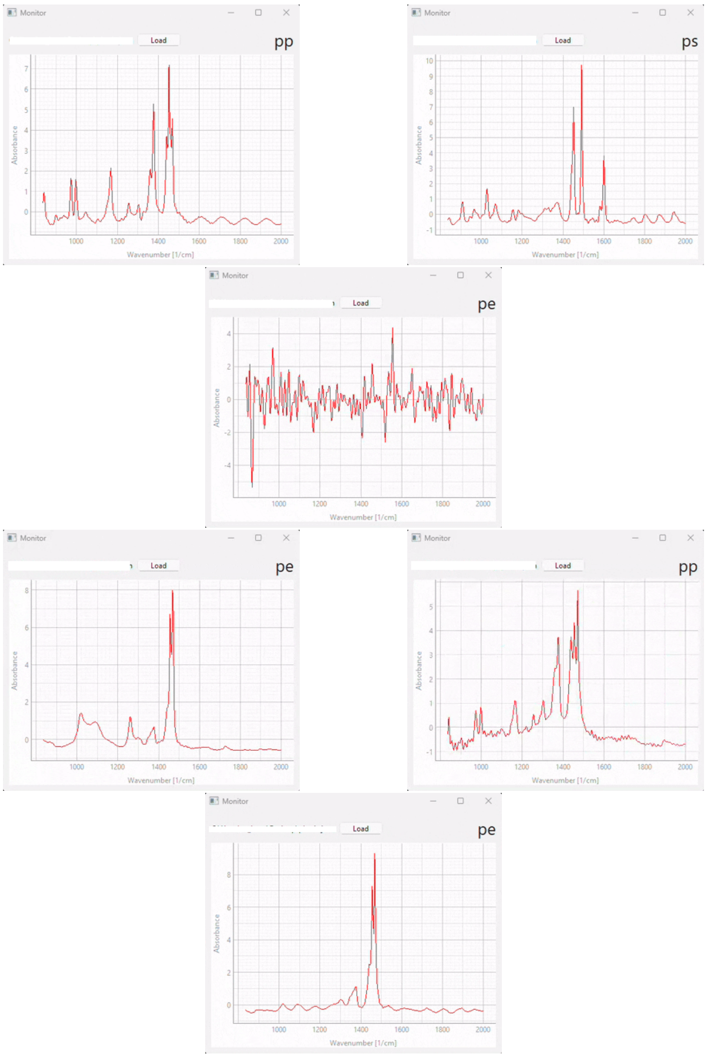


Fig. 4.11: Snapshots of real-time plastic classification using MIR spectroscopy

4.4.2 Near-Infrared Spectroscopy

Near-Infrared (NIR) spectroscopy between 800 nm to 2500 nm (12500 cm^{-1} to 4000 cm^{-1}) is widely used for rapid, non-destructive, and high-throughput plastic identification, particularly in recycling and sorting facilities. Unlike Mid-IR, which excites the fundamental vibrations of bonds, NIR light excites overtones (multiples of the fundamental frequency) and combination bands (sums or differences of two or more fundamental frequencies). For plastic samples, the overtone of the C-H stretching region is the dominant signal (Figure 4.12). The resulting NIR spectra are often broad and heavily overlapping, making direct visual interpretation difficult. This makes near-IR spectroscopy an ideal showcase for machine-learning based polymer identification.

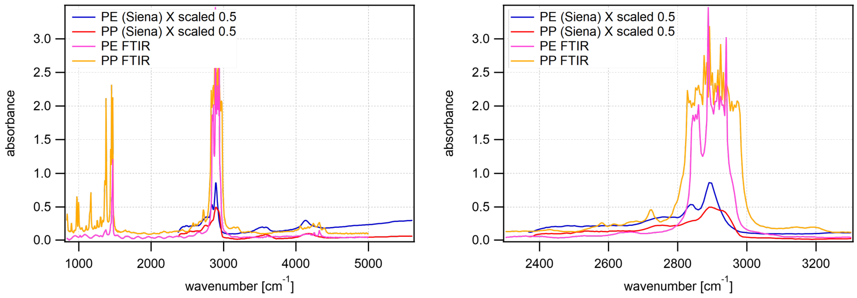


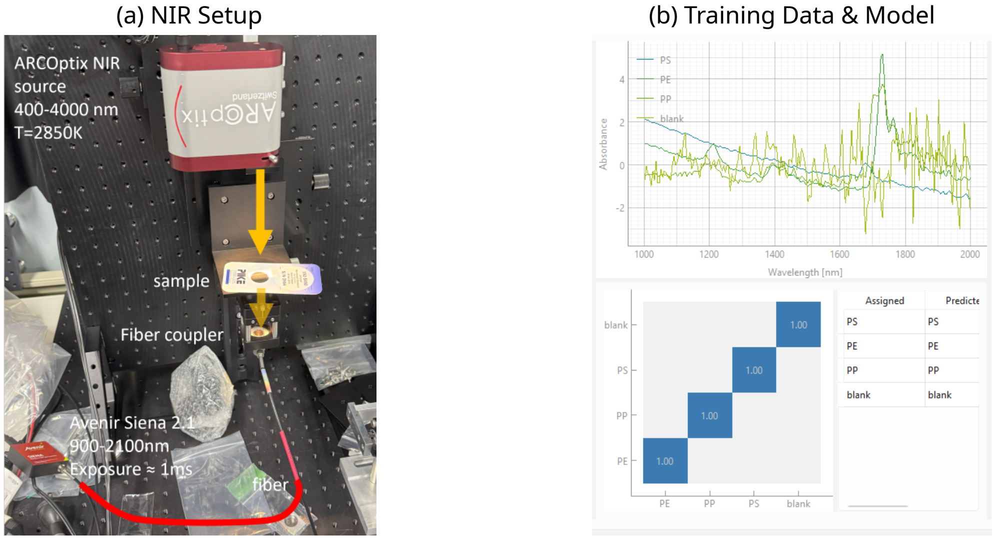
Fig. 4.12: Comparison of near-IR (blue and red) and mid-IR (pink and orange) spectra of plastic samples. The near-IR spectra have been scaled by a factor of 1/2 along the x-axis.

The measurement setup is shown in Figure 4.13 (left). Analogous to the *mid-IR experiment* (page 54), absorbance spectra were collected in transmission geometry and the transmitted near-IR light was introduced into the spectrometer using a fiber. The exposure time was around 1 ms, sufficient for high-quality spectra due to the high absorbance of C-H bonds even at the second harmonic (first overtone). For training the SVM classifier (Figure 4.13 right),

- spectra were cropped between 1000 nm and 2000 nm
- *SNV scaling* (page 36) was applied
- a blank spectrum (no sample in the beam path) was included in the training set, which consists of only four spectra (PS, PP, PE, blank) in total.

Note

This is a (deliberately) minimal training set to demontrate the robustness and performance of the SVM classifier. For a real-world model, more spectra would be included.


(a) NIR Setup

(b) Training Data & Model

Assigned	Predicte
PS	PS
PE	PE
PP	PP
blank	blank

Fig. 4.13: Plastic Classification by Near-IR Spectroscopy

Figure 4.14 displays snapshots of real-time classification of different plastic samples using the trained model. While performance is excellent,

- some samples (especially PS) suffer from high nonspecific absorbance / scattering in the□near-IR range, resulting in a strong non-linear baseline. This baseline can mislead the classifier and interfere with scaling.

- the transmission geometry is very limiting since thicker or colored samples will not transmit enough near-IR light for successful classification

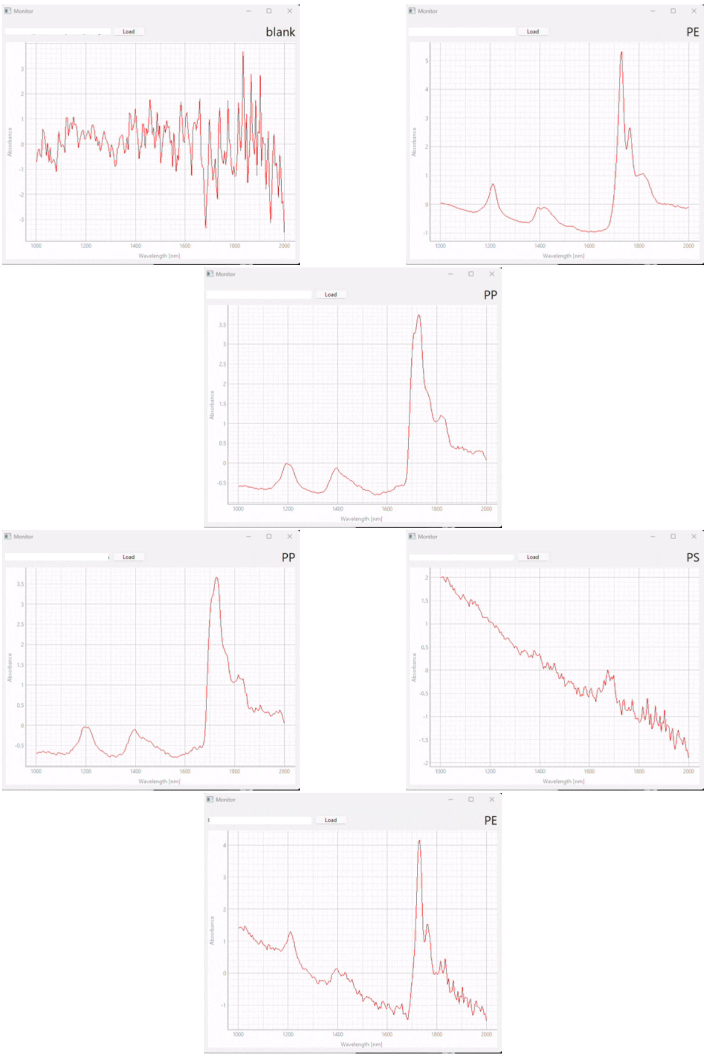
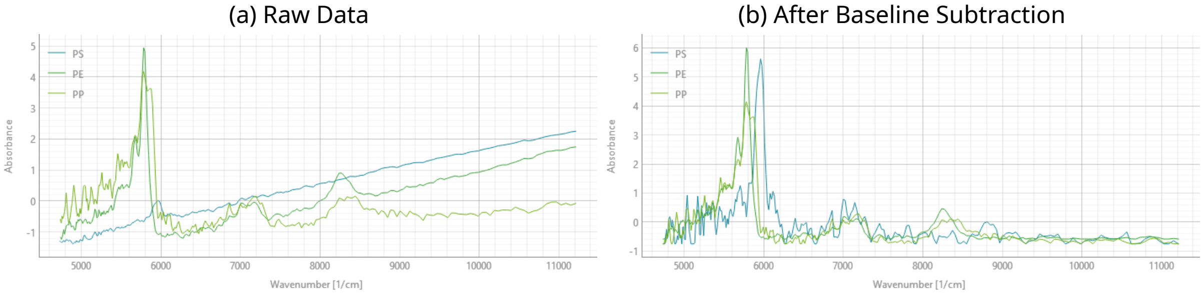


Fig. 4.14: Snapshots of real-time plastic classification using near-IR spectroscopy

Using the *baseline subtraction* (page 35) preprocessing step can remove the non-linear baseline - the result is displayed in Figure 4.15. This accentuates the absorption peaks and enables classification even in the presence of non-specific absorbance or strong scattering.


(a) Raw Data

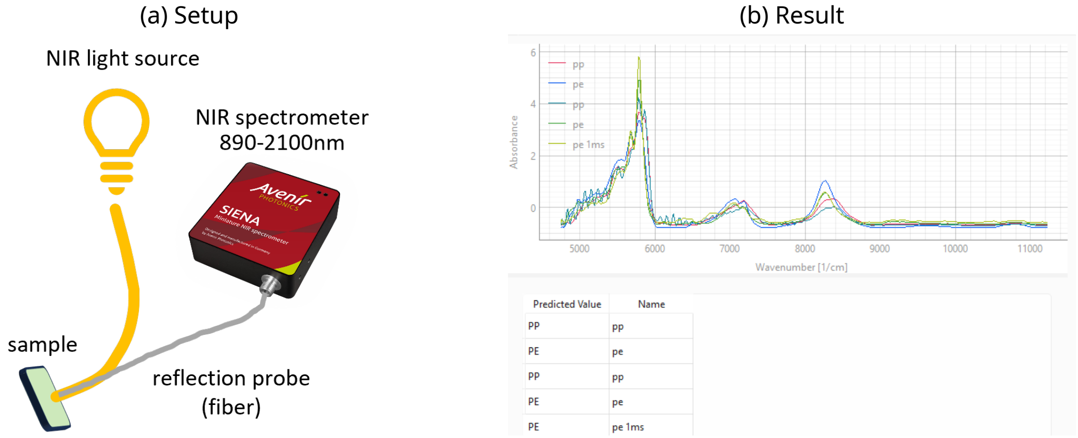
(b) After Baseline Subtraction

Fig. 4.15: NIR Classification - Baseline Subtraction

To benchmark the classifier under more realistic conditions,

- the classifier was trained using spectra collected in *transmission* after baseline subtraction (the same four spectra used in Figure 4.13)
- the classifier was evaluated using near-IR *reflections* from the plastic sample surface using a VIS-NIR fiber probe (Figure 4.16 left).

The result is displayed in Figure 4.16 (right)[1]. Baseline subtraction permits the SVM classifier to solely focus on the chemical information contained in the absorption peaks, resulting in a model with general applicability for plastic identification, independent of the collection geometry. Despite being trained on only four spectra, overfitting was avoided, as demonstrated by validating the classifier using spectra that were not only obtained from samples different from the training set but also recorded under drastically different experimental conditions.


(a) Setup

(b) Result

Predicted Value	Name
PP	pp
PE	pe
PP	pp
PE	pe
PE	pe 1ms

Fig. 4.16: NIR Classification (Reflection Geometry)

[1] The spectrum labelled *pe 1ms* was recorded in the transmission geometry.

CHAPTER

FIVE

APPENDICES

5.1 Fast Fourier Transform (FFT) Applied to FTIR Data

This section explains - mostly for educational purposes - how to extract spectra from space or time-domain interferogram data from a Fourier Transform Infrared spectrometer.

Figure 5.1 (left) displays a double-sided interferogram. The x-axis displays the optical path difference (OPD) - the travel distance of the interferometer's mirrors in *meters*. The right panel displays the shows burst around the region of zero OPD, where maximum interference is produced by the instrument.

Note

This is the data as delivered by an *ARCoptix* (page 13) FTIR instrument.

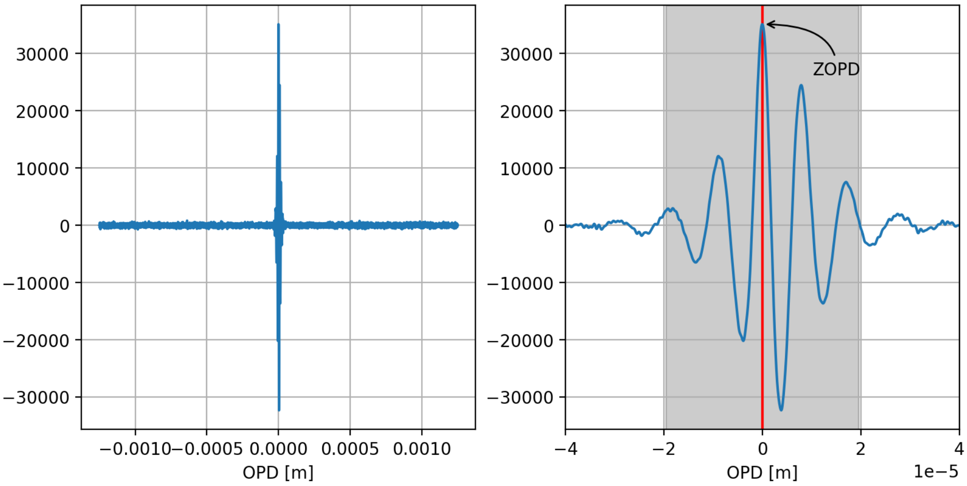


Fig. 5.1: Interferogram (left) and zoom into the ZOPD region (right)

Extracting spectral information from this data involves the following steps:

1. (optional) padding the interferogram. Padding in the space domain is equivalent to interpolation in the wavenumber domain and can be done to increase the spectral resolution.
2. preparing phase-correction data
3. extracting the sample spectrum from the phase-corrected interferogram
4. (optional) calculating absorption or transmission spectra using reference spectra

The spectrum, $B(\nu)$, is obtained by taking the complex Fourier Transform of the interferogram, $I(\Delta)$:

$$B(\nu) = \int_{-\infty}^{+\infty} I(\Delta) e^{-i2\pi\nu\Delta} d\Delta$$

Where:

- $I(\Delta)$ is the interferogram as a function of optical path difference (Δ).
- ν is the wavenumber.

5.1.1 Phase Correction

In an ideal Fourier Transform (FT) system, the interferogram (the raw signal collected by the detector) should be perfectly symmetric around the Zero Path Difference (ZOPD) point, which is where the two optical paths in the interferometer are exactly equal. However, real-world FTIR instruments introduce phase errors ($\theta(\nu)$) due to several factors, primarily:

- Instrumental imperfections: The optical components (like the beamsplitter material) have wavelength-dependent refractive indices (dispersion), which means different wavelengths travel through the material at slightly different speeds.
- Sampling/Electronics: Minor offsets between the ZPD and the first data point recorded, or electronic filtering effects.

The phase correction method used here is the Mertz[39] method, a multiplicative correction method that works in the frequency (wavenumber) domain. It estimates the phase error and then removes it from the full measured spectrum.

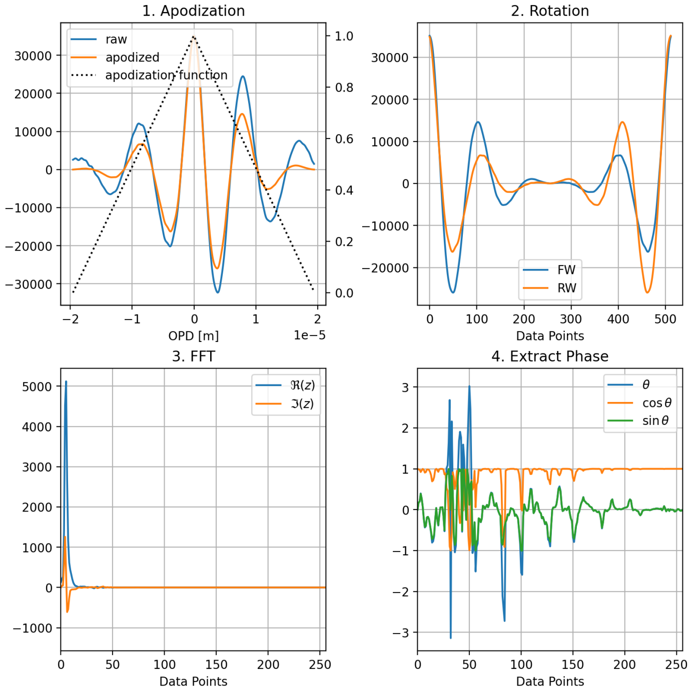


Fig. 5.2: Phase Correction

The method relies on the assumption that the instrumental phase $\theta(\nu)$ is a slowly varying function of the wavenumber. This allows the phase to be accurately determined from a small, highly symmetric region of the interferogram around the center burst (ZOPD) where the signal-to-noise ratio is highest (gray shaded region in Figure 5.1).

[39] https://opg.optica.org/ao/abstract.cfm?uri=ao-2-12-1332#Abstract

- extract a small region centered on the ZOPD (Figure 5.2) $I_{short}(\Delta)$
- apodize this region to avoid edge effects. Here, this is done using a triangular function to yield $I'_{short}(\Delta)$
- rotate the data to shift ZOPD data to 0
- perform the Fourier transform (FFT)
- The resulting complex spectrum is used to calculate the phase spectrum, $\theta(\nu)$, using the relationship between the real and imaginary parts:

$$\theta(\nu) = \arctan\left(\frac{\Im(z)}{\Re(z)}\right)$$

where z is the complex Fourier transform of $I'_{short}(\Delta)$

5.1.2 Extracting the Sample Spectrum

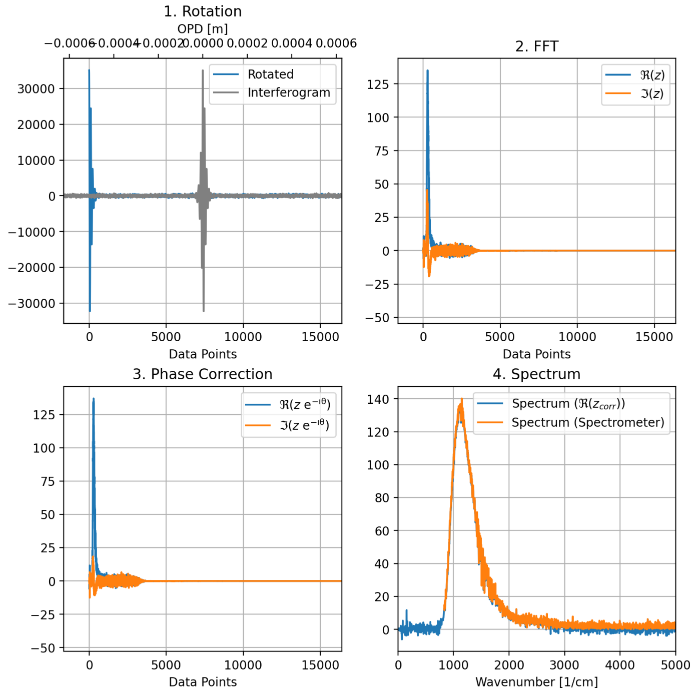


Fig. 5.3: Extracting the Spectrum

Once we have obtained the phase $\theta(\nu)$, we can phase correct the full spectrum. To this end:

- the phase spectrum $\theta(\nu)$ is interpolated to the full resolution of the final desired spectrum.
- the full interferogram is rotated to shift the ZOPD data to bin 0
- the FFT is applied to the rotated data
- the final phase correction is applied by multiplying the complex Fourier Transform of the full, single-sided interferogram by a correction term:

$$B_{corrected}(\nu) = B_{full}(\nu) \cdot e^{-i\theta(\nu)}$$

- the spectrum is the real component $\Re(B_{corrected}(\nu))$

Figure 5.3 panel 4 compares the spectrum extracted by this method (blue) and the spectrum obtained by the spectrometer (orange). While the overall shape is similar, the intensity is different. This is due to the fact that the spectrometer uses zero-padding by a factor of two to improve the spectral resolution. Since the FFT is scaled by $1/\mathrm{n}$, this will affect the amplitude as well.

5.1.3 Results

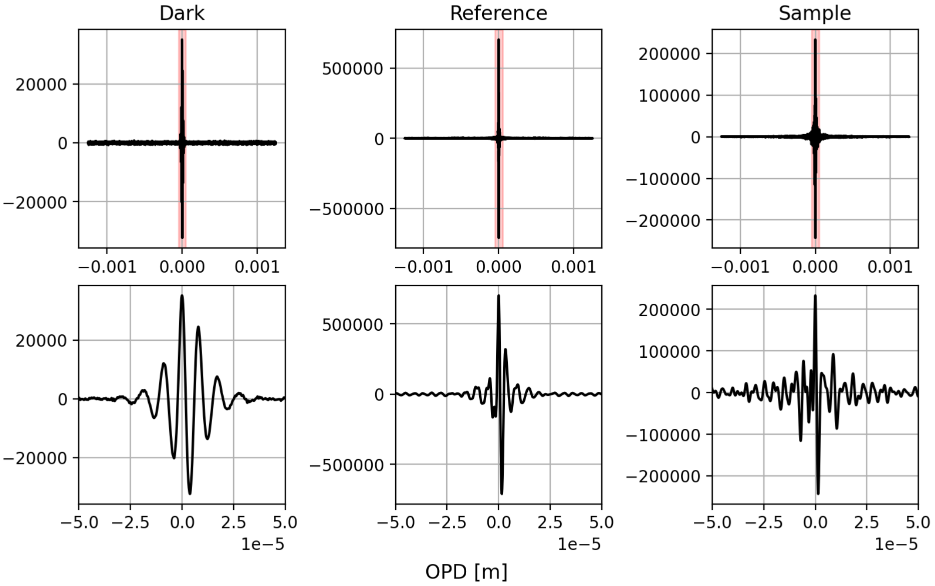


Fig. 5.4: Sample Interferograms

Figure 5.5 compares spectra that were manually extracted from interferograms (Figure 5.4) with the spectrometer’s data processing. Three spectra are shown:

- a dark spectrum where no light hits the detector
- a reference spectrum of air
- a sample spectrum of a fairly thick polystyrene sample

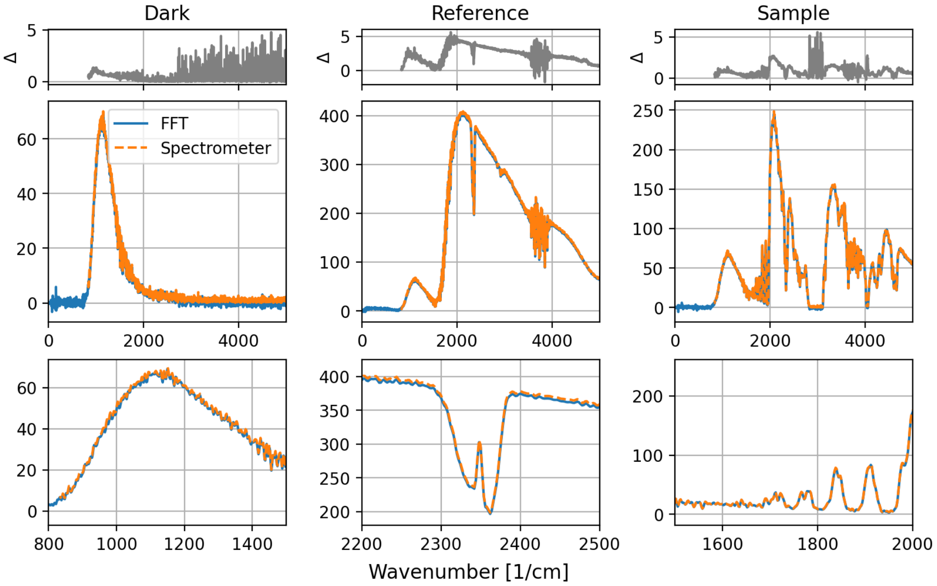


Fig. 5.5: Interferogram Analysis

For analysis:

- data was zero-padded by a factor of *2*
- phase correction data prepared as laid out in Section 5.1.1

- the full interferogram was Fourier-transformed, phase corrected, and the spectrum computed from the real component.

Overall, the agreement between manual processing and the spectrometer's result is very good. The residuals (differences between the spectra obtained by the two methods, top row of Figure 5.5) are typically very small - only a few percent of the total signal strength. Larger differences occur in regions where count rates are very low, for example in the dark spectrum at wavenumbers > 3000 cm^{-1} or for the polystyrene sample between 2800 and 3200 cm^{-1}.

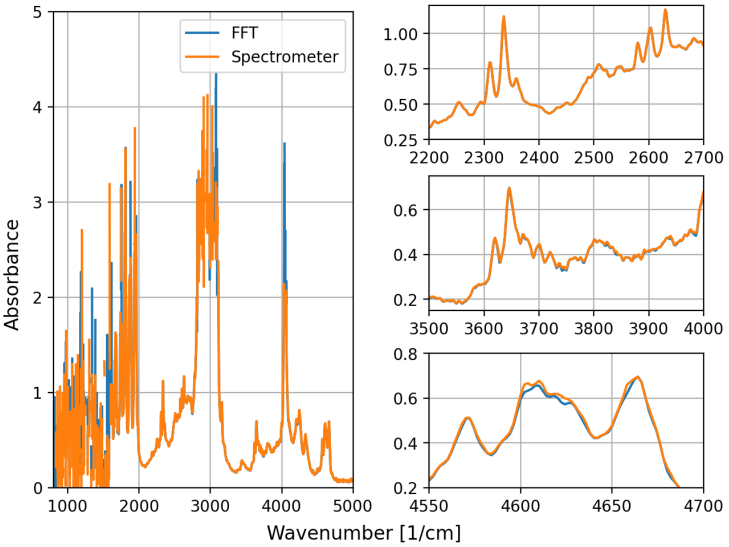


Fig. 5.6: Absorbance Spectra

Figure 5.6 shows an absorbance spectrum $\mathrm{A}(\nu)$ calculated from the raw data

$$A(\nu) = -\log_{10}\frac{I_S(\nu) - I_B(\nu)}{I_R(\nu) - I_B(\nu)}$$

where:

- $\mathrm{I_S}(\nu)$ is the sample spectrum
- $\mathrm{I_R}(\nu)$ is the reference spectrum
- $\mathrm{I_B}(\nu)$ is the background (dark count) spectrum

Again, agreement is very good except for regions of high absorbance. In these regions, even small numerical differences will be emphasized due to division and application of the logarithm. The right panels of Figure 5.6 show a comparison of key spectral regions - generally, agreement is excellent.

5.1.4 An Annotated Example

This section contains Python sample code to perform interferogram analysis. It assumes that numpy[40] is available.

Loading *CSV* Data

This snippet loads .csv data into the opd and y *numpy* arrays.

```
data_sp = np.loadtxt("data.csv", skiprows=1, delimiter=',')
opd, y =  data_sp[:, 0], data_sp[:, 1]
```

[40] https://numpy.org/

Padding

Here, we (optionally) pad the data by `fillFactor`. This is equivalent to increasing the scan range, hence the opd array now is a array of twice the number of points with twice the range. The y intensity data is padded symmetrically by appending zeros to the start and end.

```
opd = opd * fillFactor
opd = np.linspace(opd.min(), opd.max(), len(opd) * fillFactor)
y = np.pad(y, pad_width=(int((fillFactor - 1) / 2 * len(y)),), mode='constant')
```

Phase Extraction

First, we obtain the index of the *ZOPD*.

Next,

- we use a 512 point window to extract a small region around the ZOPD `yShort`
- we use *triangular apodization* (page 67) to prepare y_apo
- we rotate the ZOPD bin to 0 using `np.roll`
- we compute the FFT using `np.fft` and compute the phase `theta` using the `atan2` function

```
max_Y = np.argmin(np.abs(opd))

winSize = 512
xShort = np.arange(0, winSize)
yShort = y[max_Y - winSize//2 :max_Y + winSize//2]

apo_short = triangularApodization(yShort)
y_apo = yShort * apo_short
y_short_apo_rot = np.roll(y_apo[::1], winSize//2)
fft_short = np.fft.fft(y_short_apo_rot, norm='forward')
theta = np.atan2(fft_short.imag, fft_short.real)
```

Calculating the Spectrum

First, we interpolate the phase information to the full length of the (padded) spectrum.

```
theta_full = np.interp(np.linspace(xShort[0], xShort[-1], len(opd)), xShort, theta)
```

Next, we calculate the spectrum:

- use `np.roll` to rotate
- perform the FFT
- apply the phase correction by multiplying the real part of the FFT by exp$(-i\theta(\nu))$
- calculating the spectrum yy as the real part of the phase corrected component.
- truncate this to the length of half of the OPD since (after phase correction) the spectrum is now symmetric

```
#alternatively, apply apodization here, eg
#y_apo = y * triangularApodization(y)
y_apo = y
y_full_apo_rot = np.roll(y_apo[::1], -max_Y)
fft_full = np.fft.fft(y_full_apo_rot, norm='forward')

yy = (fft_full * np.exp(-complex(0,1)*theta_full)).real[0:len(xx)]
```

Calculating the Wavenumber Axis

Finally, we need to calculate the wavenumber axis. First, we calculate the wavenumber increment dx in cm^{-1} and fill a numpy array xx using dx as the step size.

```python
dx = 1/(opd.max() + np.abs(opd.min())) / 100
xx = np.linspace(0, len(opd)//2 * dx, len(opd)//2)
```

Apodization

A triangular apodization function for data y can be calculated using the following function

```python
def triangularApodization(y:np.ndarray):
    max_Y = np.argmax(y)
    x = np.arange(0, len(y))
    apo = 1-np.abs(x - max_Y) / (1 * len(x[max_Y:]))
    apo[apo < 0] = 0
    return apo
```

Alternatively,

- the Norton-Beer[41] package contains a number of functions commonly used in FTIR analysis
- standard windowing functions (Hanning etc.) will work as well.

[41] https://github.com/konstntokas/norton_beer

CHAPTER

SIX

WHAT’S NEW

6.1 TII Spectrometry 1.0.0 (*Bittersuite*)

This is the initial public release of **TII Spectrometry**.

TOKYO INSTRUMENTS

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