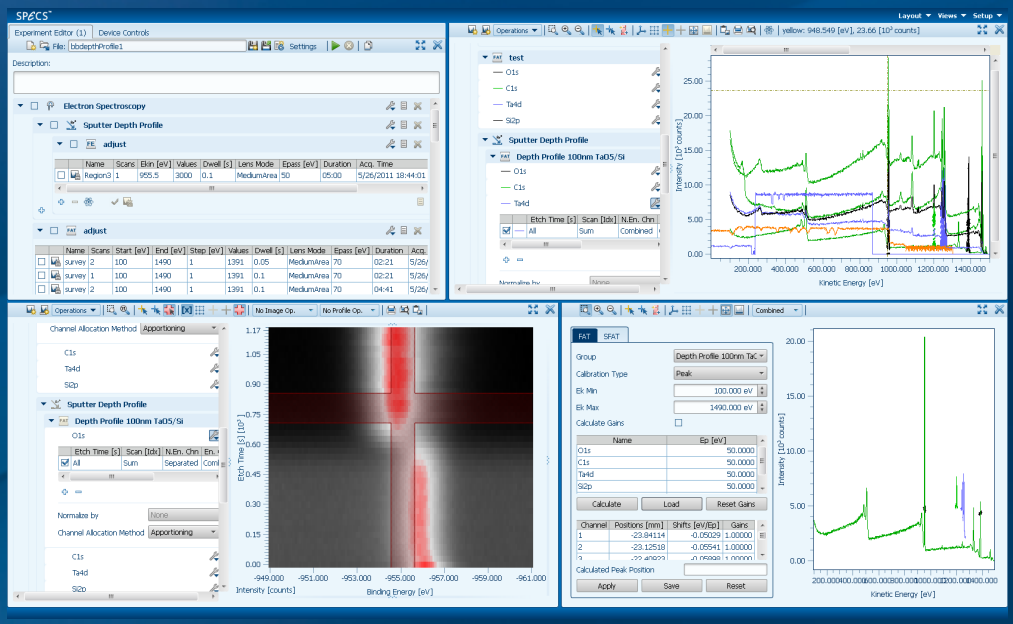
SpecsLab Prodigy

Quick Guide



SPECS™

User Manual | March 25, 2022

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SPECS User Manual

SpecsLab Prodigy—Quick Guide

March 25, 2022

SPECS order number reference: –

Table of Contents

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Chapter 1 – Installation

Installation of SpecsLab Prodigy involves two steps:

1. Installing SpecsLab Prodigy itself.
2. Installing the licenses and configuring devices with the SpecsLab Configuration Tool.

Upgrading the software and system uses essentially the same procedures:

- If you only want to upgrade SpecsLab Prodigy, you can run the new installer. The configuration of the system remains unchanged.
- If you change the configuration of your system, you can run the SpecsLab Configuration Tool to add new devices and features.

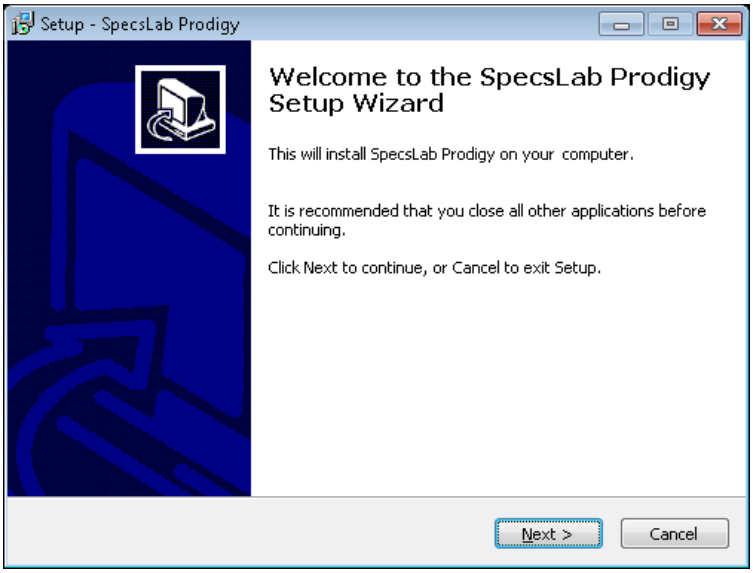
This chapter guides you through the complete procedure to obtain a new installation for a working system with an example configuration.

1.1 Installer

The installation program copies the necessary files for SpecsLab Prodigy onto your computer.

To run the installation:

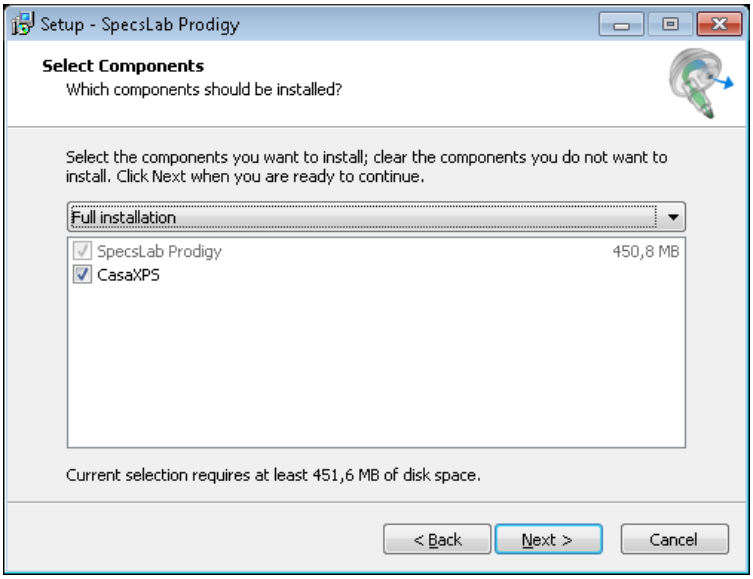
1. Start the installer by double-clicking the installer file—the filename has the general form SpecsLab Prodigy-x.xx-ryyyyy.exe.
2. The installation starts with a Welcome page. Click *Next* to continue.



3. Read the information on the page. Click *Next* to continue.
4. Select the components to be installed:
   - SpecsLab Prodigy—The SPECS data acquisition package (mandatory).
   - CasaXPS—Software for analyzing and evaluating XPS spectra.

Note

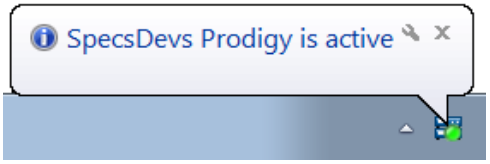
CasaXPS has its own installer. If this is available, it is started from the SpecsLab Prodigy installer.



You can select *Custom* from the drop-down list to select individual components for installation. For most purposes, the full installation provides the necessary functionality.

5. Click *Next* to continue
6. Check the box if you want a desktop icon for SpecsLab Prodigy, then click *Next* to continue.
7. Click *Install* to start the installation.

The installer will now install SpecsLab Prodigy. As part of this procedure, the SpecsDev Supervisor will start. This is a small utility that appears in the taskbar to show the status of the service SpecsDevs. SpecsDevs needs to be running in order to start SpecsLab Prodigy.



You can move the SpecsDevs Supervisor into the taskbar tray if desired. Right-clicking the utility opens a context menu, which allows you to stop and restart SpecsDevs, if necessary.

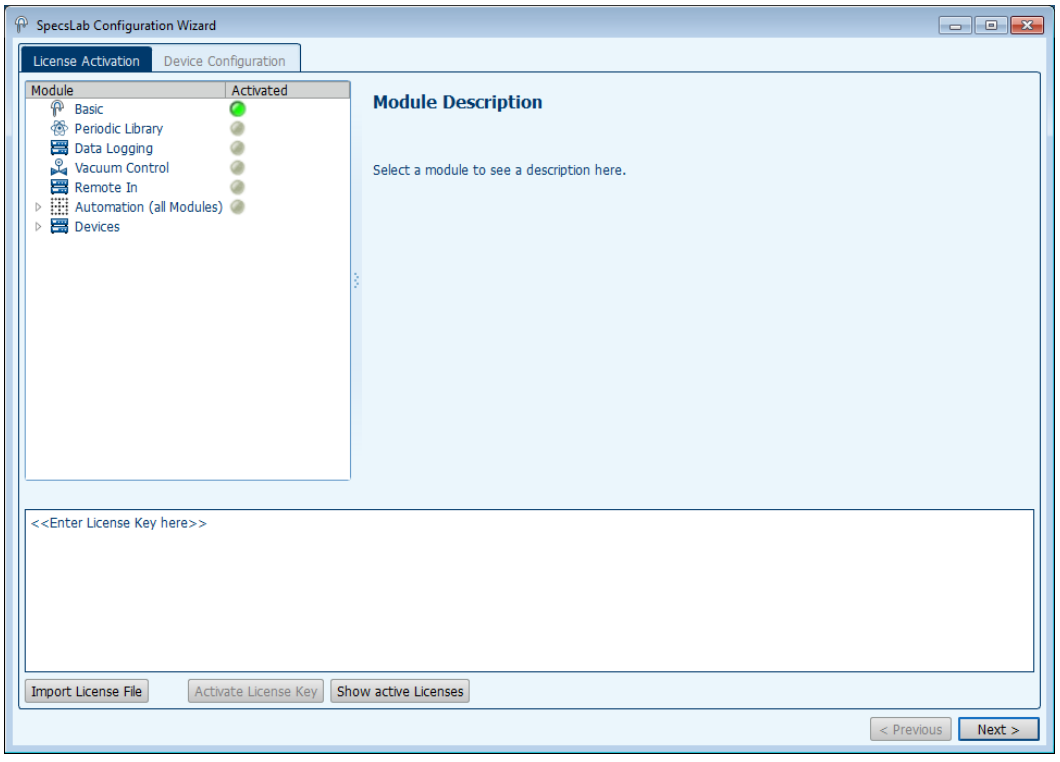
At the end of the installation, the SpecsLab Configuration Tool wizard will start.

1.2 Adding Licenses

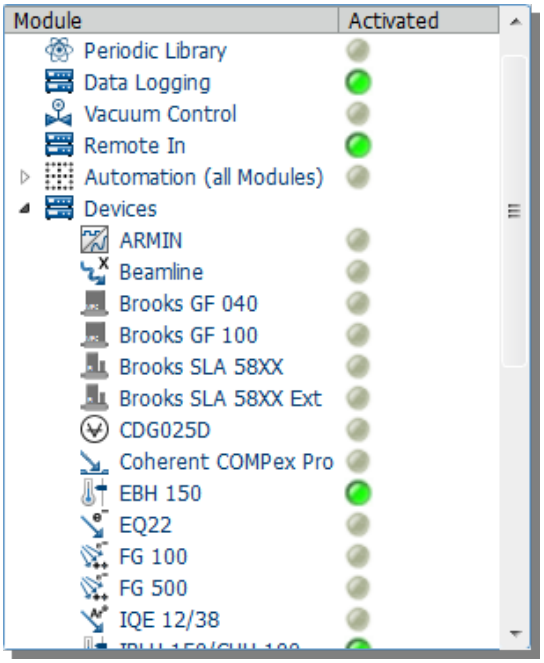
SpecsLab Prodigy uses a modular licensing system. In the Basic configuration, the following software features are available:

- PHOIBOS analyzers.
- Dummy devices that provide excitation sources for an experiment (software simulated).
- Basic facilities for acquiring and evaluating data.

Additional modules of SpecsLab Prodigy can be activated by using the respective licenses. The first page of the SpecsLab Configuration Tool wizard allows you to enter the licenses for each of the modules:



As soon as a license is added, the licensed module will be marked with a green indicator:



There are two methods for entering the licenses, as described below.

To enter a license directly:

1. Copy the license key(s), e.g. from an email from SPECS, and paste it into the pane in the lower part of the window.
2. Click *Activate License Key*. The license keys will be read and the corresponding modules enabled.

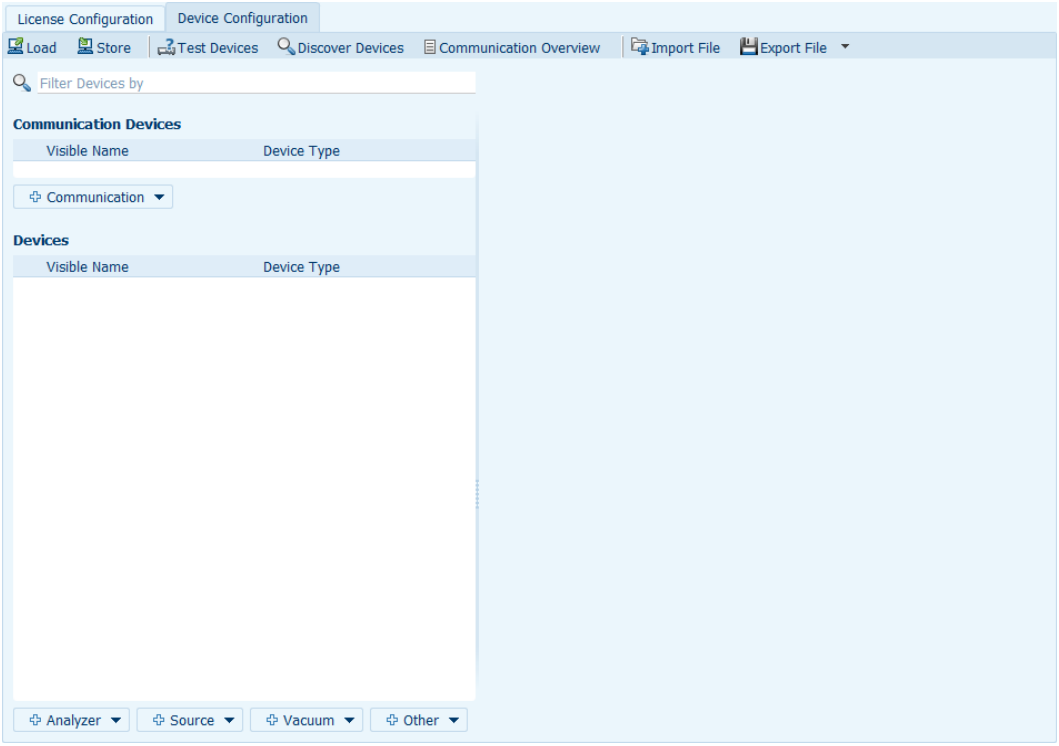
To use a license file:

1. Click the *Import License File* button. A file browser will open.
2. Select the license file. This has a .lic extension.
3. Click *Open*. The contents of the license file will be added to the licenses pane.
4. Click *Activate License Key*. The license keys will be read and the corresponding modules activated.

Check that all of your features have been activated, then click *Next* to move on to the next page in the wizard.

1.3 Configuring Devices

The second page in the wizard allows you to add the devices on your system. This provides SpecsLab Prodigy with details of which devices are present, together with their operating parameters. You can also test the connection to the instrument to make sure that it will work when SpecsLab Prodigy starts.



The setup is generally straightforward, but may be different for each device. Describing each possibility is beyond the scope of this guide—if necessary, please refer to the user manual for the device. The following procedure is an example that describes how to configure a PHOIBOS energy analyzer and an X-ray source.

Note

You can start the SpecsLab Configuration Tool at a later time to change the configuration without reinstalling SpecsLab Prodigy.

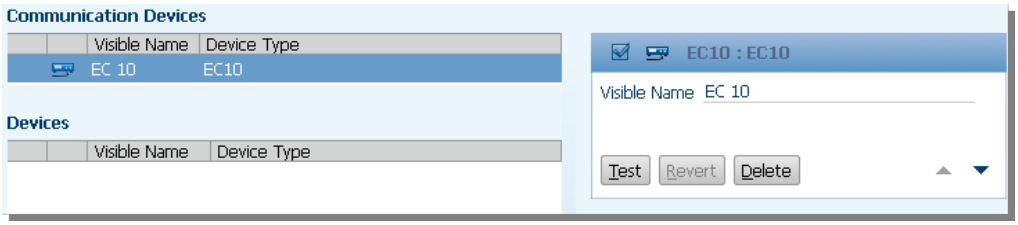
Note

In each step of the following procedure, you need to test the device. For configurations with many devices, you can use the Test Devices in the toolbar to test all devices in a single action.

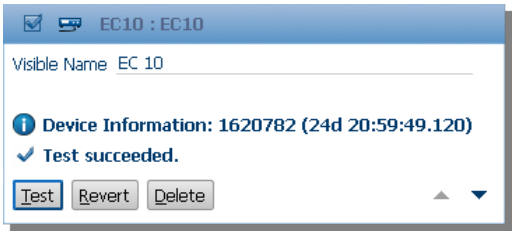
1.3.1 Setting up EC 10

Some SPECS instruments use CAN as a communication protocol. These are accessed using the EC 10, an ethernet-to-CAN converter. You need to set up the EC 10 in order to use the analyzer and source:

1. Click the button Communication and select *EC10* from the menuto add the new device to the *Communication Devices* section. Its properties will be displayed in the right pane.



2. Make sure the EC 10 is switched on and connected.
3. Click *Test*. SpecsLab Configuration Tool will make a connection to the EC 10 and check that it is working.



If there is a problem, an error message will appear – in this case check the following:

- The EC 10 is switched on and connected as described in the PHOIBOS manual.
- The network settings are correct. Click ▼ to see these settings. If you have changed The settings in the EC 10, enter the correct IP address (do not change the port number without instructions from SPECS support). The *Revert* button will undo any changes.

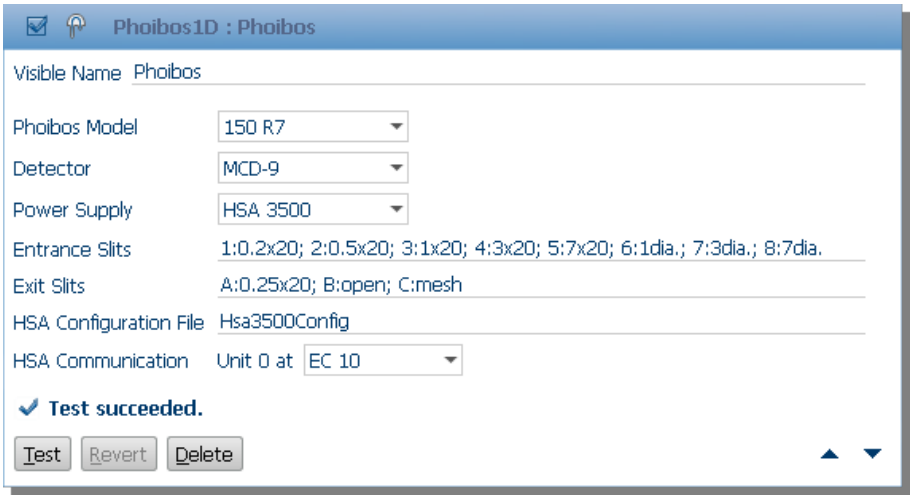
1.3.2 Setting Up the PHOIBOS Analyzer

With the communication interface working, you can add the analyzer.

Note

If you have a PHOIBOS analyzer with a CCD detector, you need to install the camera driver. Please see the detector manual for details.

1. Click the button Analyzer and select an analyzer:
   - *PHOIBOS1D* for analyzers fitted with one-dimensional detectors, i.e. channel electron multipliers or 1D delay lines.
   - *PHOIBOSND* for analyzers fitted with multi-dimensional detectors, e.g. 2D CCD detectors.
2. Edit the following fields:
   - *Visible Name*: The name of the device as it will appear in SpecsLab Prodigy.
   - *PHOIBOS Model*: Select the model of your analyzer. This will also determine the slit settings.
   - *Detector*: This ensures that SpecsLab Prodigy correctly processes acquired data, particularly when dealing with multi-channel data.
   - *Power Supply*: This will also select the correct HSA configuration file.
   - The other settings are shown for reference and should only be changed by SPECS support.



3. Click *Test* to check the correct operation of the power supply. Provided the EC 10 passed the communication test and the HSA power supply is switched on, this test should be successful. If not, check that the settings are correct.

1.3.3 Setting Up the Excitation Source

You need to define an excitation source. At the very least, this allows you to define the experimental conditions (e.g. photon energy) for the experiment. There are two possibilities

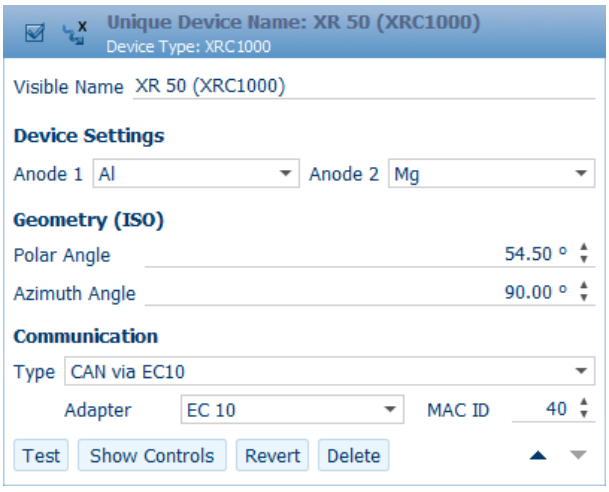
- Dummy control. If you do not have a SPECS X-ray source, you can set up a dummy which simulates the source in the software.
- Control of the SPECS power supply. This switches on the source as part of the experimental configuration.

Note

If using an electron or UV source, you can set up a dummy device with the EQ 22 and UVS devices respectively. There are also devices for controlling sources with monochromators and for beamlines at synchrotrons.

The following description applies to both dummy sources and control of a power supply.

1. Click the button Source and select *XRC 1000* from the menu.
2. Edit the following fields as necessary:
   - *Visible Name*: The name of the device as it will appear in SpecsLab Prodigy.
   - *Anode 1*, *Anode 2*: Select the material for the anodes. SpecsLab Prodigy will use the energy of the excitation line to calculate binding energies.
   - *Polar Angle*, *Azimuth Angle*: These angles specify the orientation of the source within the chamber coordinate system. This information can be used for data evaluation purposes.
3. Click to display the Communication settings, if not already visible.



4. If you wish to use a dummy source, click *Type* and select *Dummy* from the drop-down menu. The other communication settings will then disappear. For a source controlled by CAN via EC 10, the communication settings are correct for the standard configuration of the instrument and should only be changed by SPECS service engineers.
5. Click *Test* (this option is not available for dummy devices). SpecsLab Configuration Tool will locate the XRC 1000 and make sure it is working properly.

Chapter 2 – SpecsLab Configuration Tool

The SpecsLab Configuration Tool runs as part of the installation procedure. You can start the SpecsLab Configuration Tool at any time later in order to change the configuration. Although the workflow is essentially the same as during the installation, there are some small differences in the standalone application:

- It does not run as a wizard. You can switch freely between the two tabs, and either add licenses or configure devices, or both.
- There are additional options in the Device Configuration tab for saving/loading and import/export.

The sections in this chapter provide an overview of all the features in the SpecsLab Configuration Tool, as well as a short description of the licensing system. For a step-by-step usage example also refer to section 1.2 and 1.3.

To start SpecsLab Configuration Tool:

- From the programs in the Start Menu select *SPECS SpecsLab Prodigy/SpecsLab Prodigy Configuration*.

Note
SpecsLab Configuration Tool requires Administrator rights in order to run.

2.1 Module Licenses

SpecsLab Prodigy uses its licensing system to enable various software modules. Each module has a short description of its function. It will be shown as you select the module on the tab *License Configuration*.

If you are interested in obtaining a license for a module, please contact SPECS support.

Note
When installed, the Online Help contains details about the selected modules.

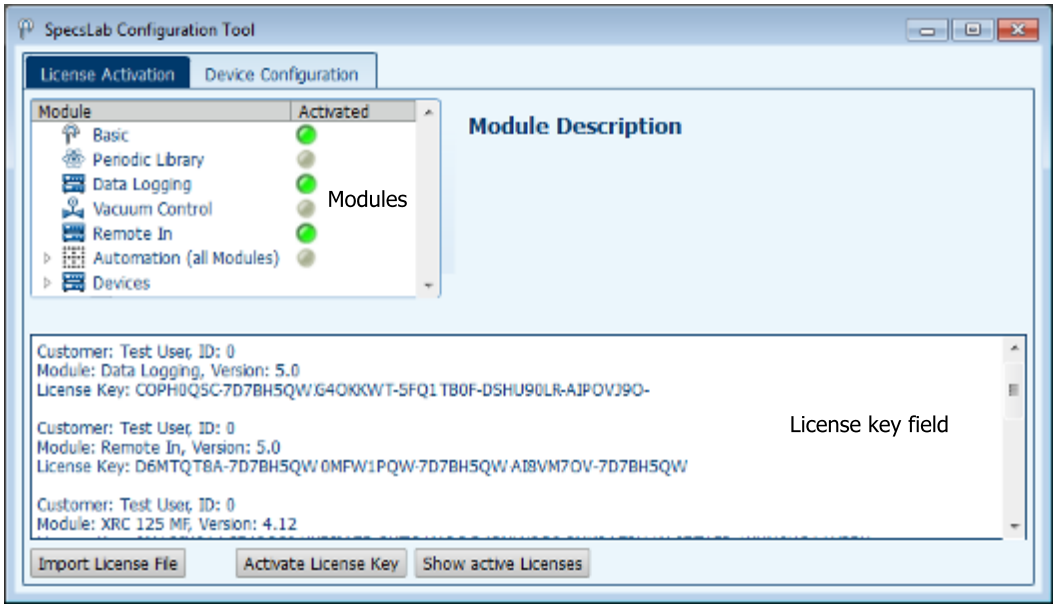
Each license contains the following three lines:

- Customer: name of customer, with an ID code
- Module: The module to be licensed.
- Key: The license code.

All licenses are stored in a text file at the following location:
C:\ProgramData\SPECS\SpecsLab Prodigy\LicenseManager

2.2 License Activation

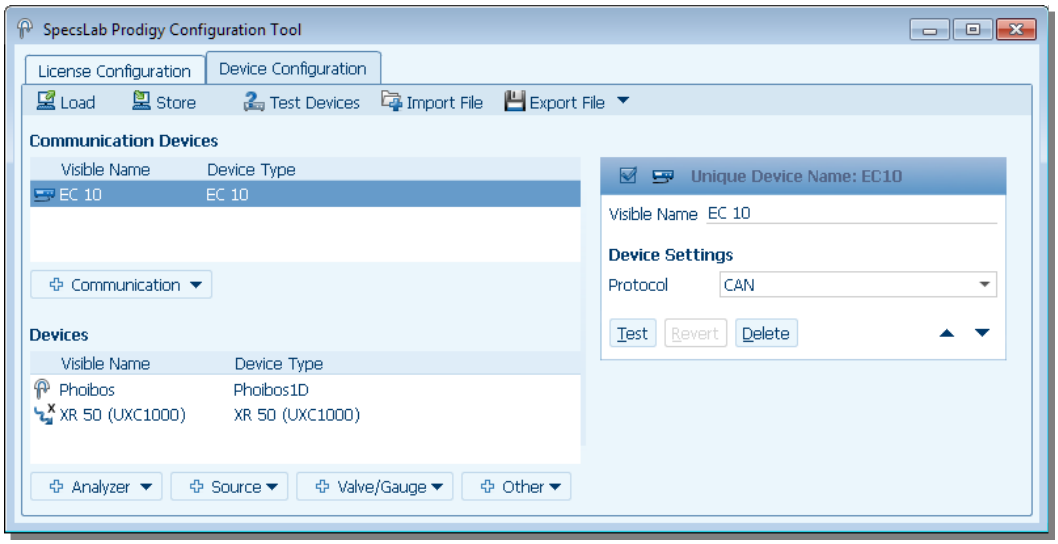
The License Activation tab allows you to add licenses for devices and features, as well as viewing the installed licenses. The screenshot below shows the License Activation tab. All of the features are described in the table.



Feature	Description
Modules	A complete list of all available modules. Activated modules are marked with a green indicator.
Module description	A short description of the currently selected module.
License key field	Displays the licenses that can be activated by pressing the Activate License key. You can paste a license into this region; otherwise, licenses imported from a file are displayed here. Licenses that have been activated in a previous session are not shown.
Import License File	Opens a dialog allowing you to select a license file (extension .lic). When loaded, the licenses are displayed in the license key field.
Activate License Key	Activates the licenses displayed in the license key field.
Show Active Licenses	Pops up a field showing the details of all activated licenses.

2.3 Device Configuration

The Device Configuration tab allows you to add and set up devices on your system. There are also facilities for transferring your configuration to another computer. The screenshot below shows a typical configuration. Each control and feature in the tab is described in the table.

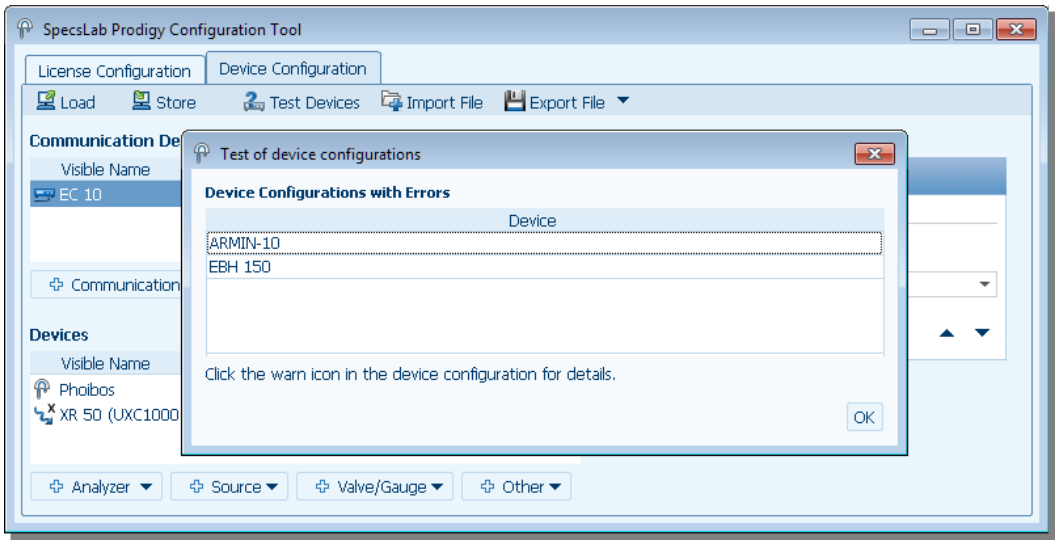


Feature	Description
Load	Loads the current configuration from the registry. Any unsaved changes you have made will be lost.
Store	Saves your configuration to the registry. This is necessary so that SpecsLab Prodigy can read the configuration.
Add Device	Contains a list of devices that can be added to the configuration.
Test Devices	Tests all Devices in the Communication Devices and Devices section. See below.
Import File	Allows you to import a configuration. Used with the Export File feature, this allows you to transfer a working configuration from one computer to another without needing to reconfigure each device again.
Export File	Exports the current configuration to a file.
Communication Devices	A list of all devices in the configuration that are used for communicating between the computer and other devices.
Devices	A list of all devices in the configuration.
Device Configuration	A field that allows you to set and test device parameters.

Test Devices

The Test Devices button allows you to run a test of all of your configured devices. If any fail the test, a dialog will appear showing which devices have a problem. You can copy these details to the clipboard for reference or send the details to SPECS via mail.

The devices which fail the test are marked with warning signs in the main window. On selecting the device, you will see some information about the nature of the problem.



Chapter 3 – Measuring a Spectrum

The Experiment Editor is used to define and run experiments.

The following procedure contains the basic steps for performing a simple scan. The Experiment Editor contains a wide range of additional features that allow you to perform more complex experiments, such as scheduling different tasks and defining templates for standard tasks. Please see the Online Help for more details.

To create a new experiment

1. Under *Create Experiment from Scratch*, click *XPS*. The Experiment Editor will show the details for an XPS experiment. Instead of XPS, you can also select options for UPS, AES and ISS experiments. The difference is the sources that are available for the experiment. The
2. Edit the experiment file name as necessary. The default is Experiment, followed by a date and time stamp.
3. Enter some text in the *Description* field. This is recorded with the data. It is valid for the entire experiment. Typical information would be details of the surface, adsorbate, etc.

3.1 Adding a Source

You need to define the properties of the excitation source. For the purposes of this description, we will use a "dummy" X-ray source. Other SPECS sources, as well as instruments such as beamline monochromators, can be controlled directly from SpecsLab Prodigy.

To add a dummy X-ray source to the experiment:

1. Click *XR50 Dummy: Operate*. A new XR50 Dummy entry box will appear in the Experiment Editor.

Note

If there is only one source available, it is automatically added to the experiment.

2. Select the desired excitation energy from the *Anode* drop-down list. This information is used to calculated binding energies. It is also stored with the data with other experimental information.
3. If desired, check the *Notify to set up device* box. Before data acquisition starts, a dialog will pop up instructing you to switch on the X-ray source with the correct parameters.
4. For further source parameters, click the ▼ button.

5. Enter desired values for the source power and high voltage as necessary.

3.2 Adding an Analyzer and Other Devices

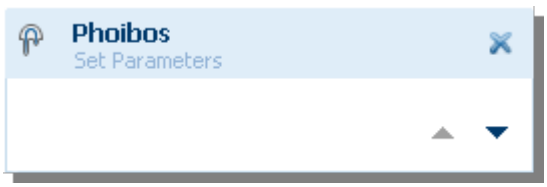
An analyzer is essential for all measurements. If you only have one analyzer, this is automatically included in the experiment. If you have additional analyzers and detectors, you can choose which one to use for the experiment.

In addition to the analyzer, you may be able to select other devices for use in the experiment. You can then set the operating parameters to be used in the experiment. Typical devices include:

- Flood gun, to be activated during a measurement.
- Manipulator, to move the sample to the measurement position.

To add an analyzer:

- Click the desired analyzer in the list of devices in the Experiment Editor. The analyzer will be activated when you start the experiment.



In addition to the analyzer, you may be able to select other devices for use in the experiment. You can then set the operating parameters to be used in the experiment. Typical devices include a flood gun, manipulator or sample heater.

Some modules are dependent on a device being defined at this point. If you have the Profiling and/ or Ramping modules, you need to add the device in order to be able to access the parameters in the module.

External devices may also be available. These allow you to record a parameter while the experiment is running. A typical example is to measure the sample current for normalizing the signal. The data from the external device can be viewed in the data browser; this also offers the facility to use the data for normalizing the signal.

Note
After the end of the experiment, the all devices are put into a safe status. The exact details of this final status are device dependent.

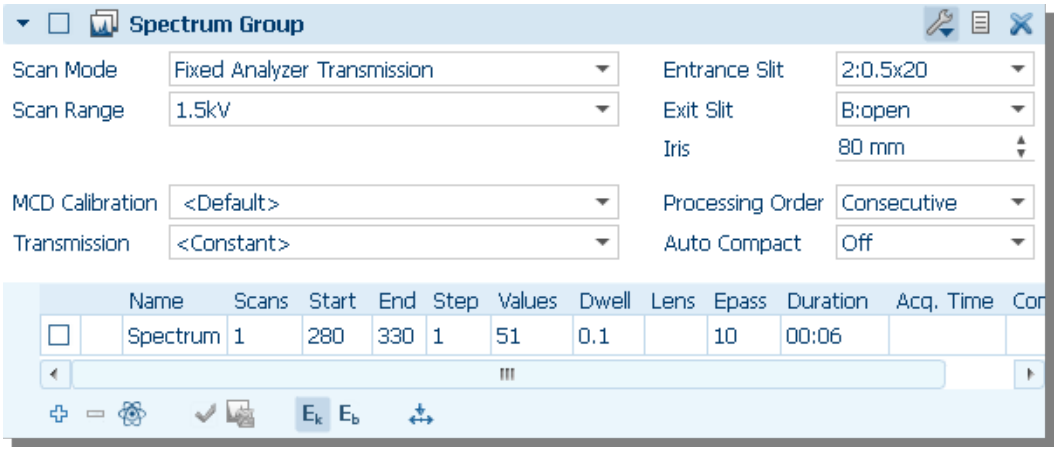
3.3 Creating a Spectrum Group

Spectrum Groups contain one or more spectra. Each spectrum is recorded using the same analyzer settings, but with different energy settings and lens modes. Within a single experimental run, you can therefore measure a number of regions in the energy range.

To create a new Spectrum Group:

1. Click the  icon next to *Add to Electron Spectroscopy*. A new Spectrum Group will be added. If a menu appears, select *Spectrum Group*.
2. Click the name ("Spectrum Group") and enter a name for the group.
3. Click the *Scan Mode* drop-down list. There will be a delay while the software connects to the HSA power supply.
4. Select *Fixed Analyzer Transmission* from the *Scan Mode* drop-down list.
5. Select *1.5 kV* from the *Lens Voltage* drop-down list. For the most accurate measurements, you should select the lowest available voltage for the energy range you want to measure. The HSA power supply manual contains more information about the available energy ranges.
6. Select a calibration file suitable for your detector from the *MCD Calibration* drop-down list. This corrects energy shifts between different measurement channels.

7. Select *Consecutive* from the *Processing Order* drop-down list. There are two options:
   - *Consecutive*—all spectra in the group will be measured consecutively.
   - *Cyclic*—depends on the number of scans defined. All energy regions are measured once consecutively. SpecsLab Prodigy then the returns to the start of the group and goes through the group, as defined for each individual spectrum. This cycles until all scans are performed.
8. Select a transmission function from the *Transmission* drop-down. Transmission functions are dependent on the slit settings.
9. Set *Auto Compact* to *Off*. Auto compacting allows you to reduce file size by discarding the information in separate channels (for multichannel detectors) or summing the data from a number of scans.
10. Set the *Entrance Slit* and *Exit Slit* entries according to the slits selected on the analyzer.
11. Set the *Iris* according to the setting on the analyzer.

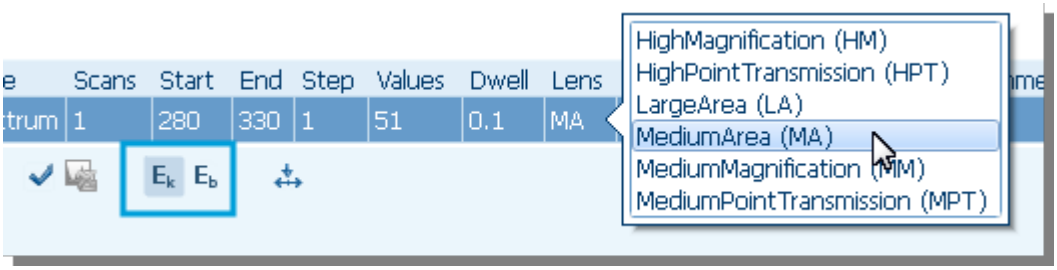


The main settings for the Spectrum Group are now complete. You are ready to define a spectrum. By clicking the  icon in the Spectrum Group, you can hide the settings you have just defined and concentrate on the details of the spectrum.

3.4 Setting Up a Spectrum

Individual spectra are defined in the table below the experiment settings. The entries in the table depend on the scan mode selected.

The *Lens Mode* opens a list that contains all available lens modes for your analyzer. This is specific to your analyzer—the modes are described in the analyzer manual.

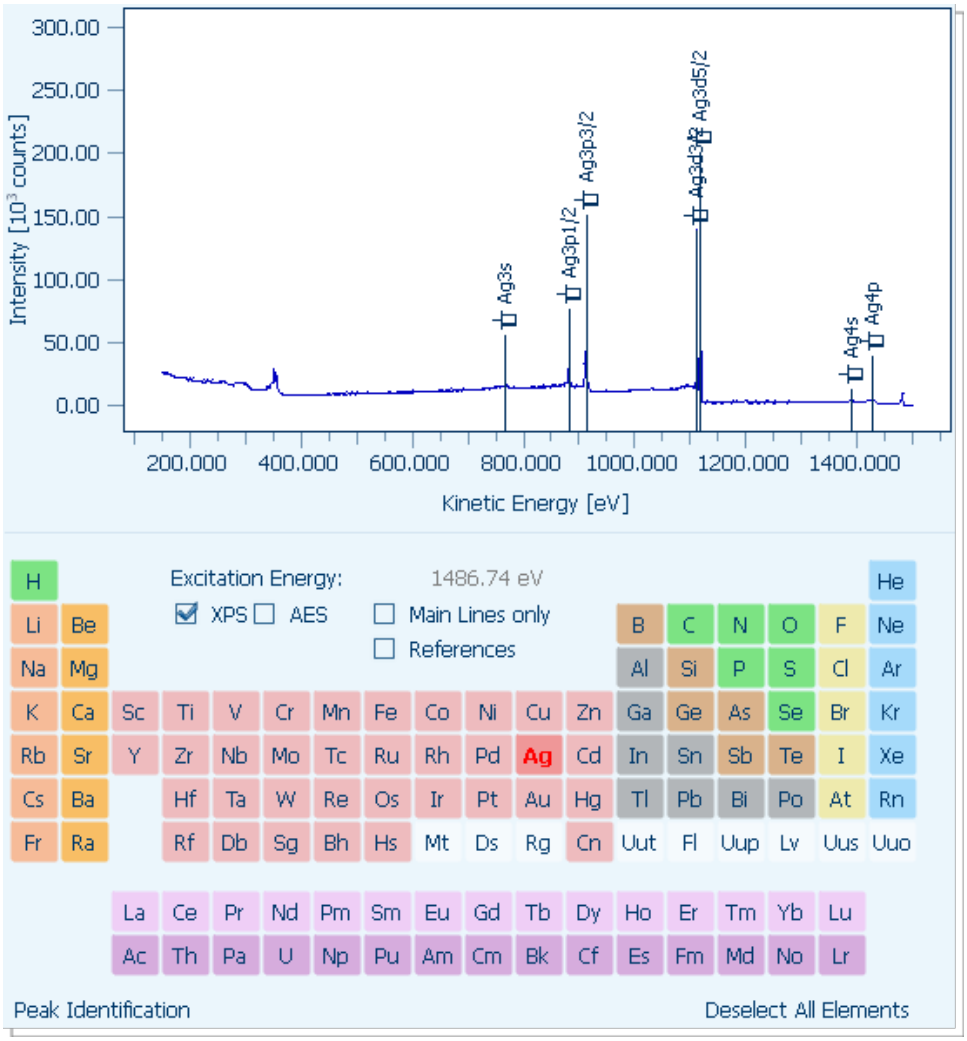


You can select kinetic energy or binding energy for the display by clicking the Ek and Eb button respectively. The binding energy is calculated from the source energy.

A particularly easy method of setting up spectra is to use the periodic table button:

- Click the icon below the spectrum group table and click an element. A menu will appear with a list of peaks that you can select. The spectrum will be set up with suggested parameters for scanning the peak.

  Remember to set a lens mode for the spectrum.



Further configuration options:

- Click the button to add another spectrum to the group. This duplicates the selected spectrum, or the last spectrum if none is selected. A new line is added to the table with the parameters for the spectrum. To remove a spectrum, first select the row in the table, then click the button. You can move a spectrum to a different position in the group using drag and drop.
- Add a data operation to the spectrum in the Plot View. The data operation is automatically performed after the spectrum is acquired.
- Add additional spectrum groups or spectroscopy experiments to the Experiment Editor in order to run many measurements in one sequence.
- Add other instruments or operations to the schedule.

3.5 Starting a Measurement

SpecsLab Prodigy performs a validation check on the experimental settings before starting acquisition. In general, small inconsistencies in the settings are automatically corrected. If there is a more serious problem in the configuration, an error message appears which tells you how to fix the problem.

To acquire specified spectra, use one of the following methods:

- Check the box in the leftmost cell for the spectrum you want to acquire. This action validates the spectrum. If you have defined additional spectra, you can also check these as you wish. Only spectra, which have been selected, will be acquired.
  Click the  button in the main toolbar.
- Select a number of spectra by holding down SHIFT (to select a range of items) or CTRL (to add the selected item) and click the spectra you want to acquire, then click  under the spectrum group.
  Click the  button in the main toolbar.

The selected spectra will be acquired.

To acquire all spectra:

1. Click the  button in the main toolbar. A dialog will appear, asking if you want to run the entire schedule.
2. Click *Yes*. All spectra will be acquired.

If you selected *Notify to set up device* when adding the source, a dialog will now appear to prompt you to switch the source on with the correct settings.

Note

Devices controlled by SpecsLab Prodigy will be automatically switched on without requiring a prompt. The status of each device is shown in the menu bar.

You can pause acquisition by clicking the icon or abort the scan with the icon. There is also the "panic button" in the menu bar which allows you to switch off all connected instruments.

After data acquisition, the spectrum is locked, as indicated by a icon. To unlock spectra:

1. Select the spectrum in the spectrum group. You can select a number of spectra by holding down the SHIFT or CTRL keys, as described above.
2. Click . There is a warning that all data will be deleted from the selected spectra. Confirm this to unlock the spectra. You can now edit the spectrum as necessary and reacquire.

3.6 Saving Data

SpecsLab Prodigy has an Autosave feature. This saves data during and at the end of acquisition. In the event of a program crash or similar interruption, you can reload the file in order to restore the settings and data. Clicking the Save icon next to the name will also save the current status of the experiment.

Clicking the arrow next to the Save icon produces a menu with the following options:

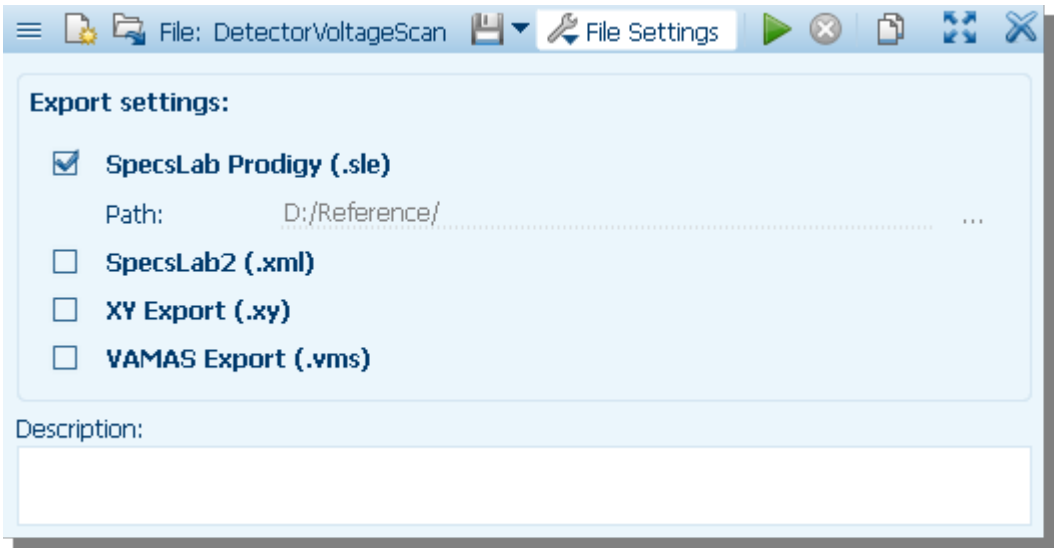
- Save the experiment.
- Save As, which opens a dialog allowing you to specify a new name and location for the experiment file.
- Duplicate the experiment, with the experiment being saved under a new automatically generated name.
- Export to various formats.

Note the following points about files:

- You can set the location by clicking *Settings* and entering a path in the field provided. Clicking the ellipsis button opens a file browser so you can select a folder.
- The default name of the file is the experiment type (e.g. Electron Spectroscopy) with a date and time stamp.
- SpecsLab Prodigy uses a binary format that contains all data and experimental details. You can export data to different formats.
- You can export individual spectra by right-clicking the spectrum in the spectrum group and selecting *Export Spectrum Data* from the context menu.

Note

SpecsLab Prodigy is able to export to the VAMAS format—see the last option in the screenshot below. Although importing from this format is also possible, not all information in the experiment will be saved for future use.



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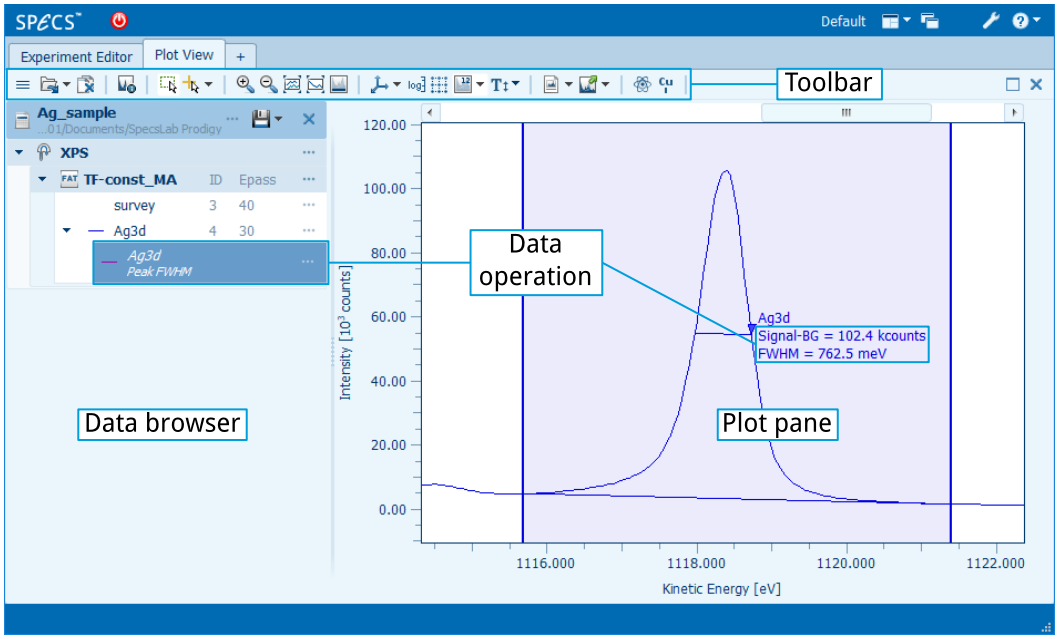
Chapter 4 – Plotting Data

The Plot View displays data acquired during an experiment. The main areas are:

- Data Browser—lists spectra and allows you to select and alter the display of data.
- Plot pane—displays spectra and data operations.
- Toolbar—provides additional controls, which primarily affect the appearance of the plot pane.



Using the data browser, you can show or hide spectra, change the display of data and perform data operations. The procedures are outlined below.

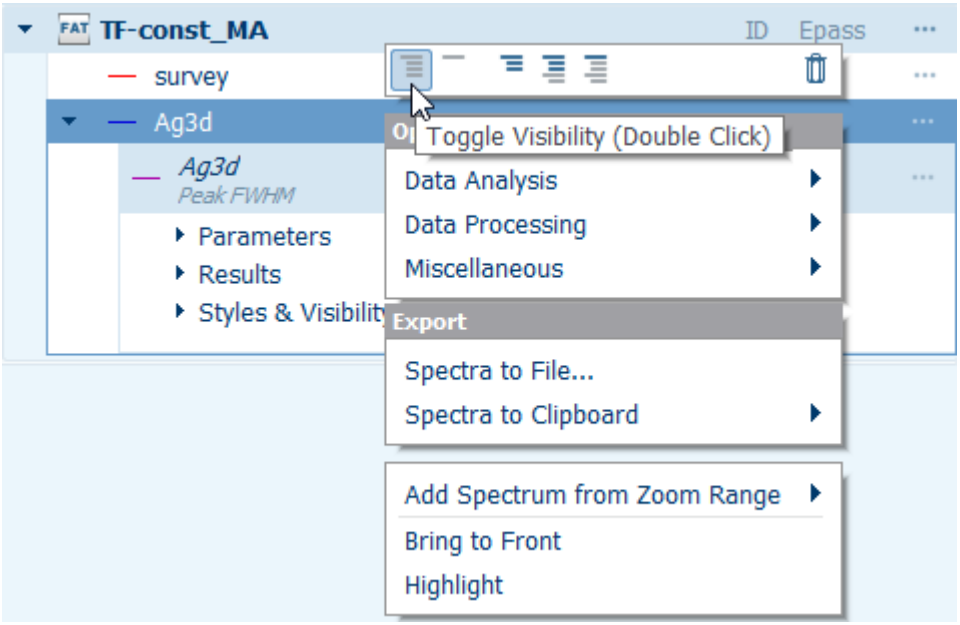
Furthermore, you can open a periodic table feature from the toolbar that helps you analyze data. A description of how to use its functions is included in this chapter as well.

4.1 Showing and Hiding Spectra

You can toggle the visibility of each spectrum in the Plot View for clarity or comparison.

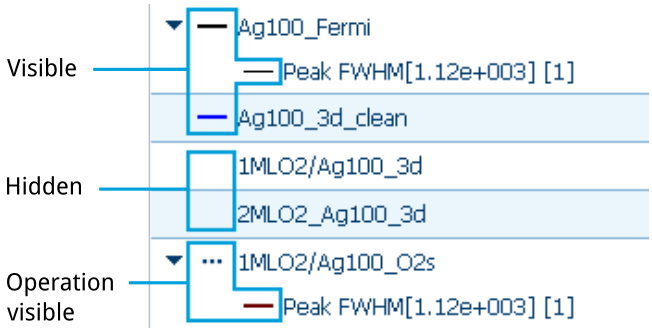
To toggle the visibility of a spectrum in the plot, use one of the following methods:

- Double click the name of the spectrum or data operation. The axes in the plot are automatically scaled to the displayed spectra.
- Right-click on the spectrum or data operation that you want to show or hide. Alternatively , click the icon ··· to the right. A menu will appear with a set of control buttons above it:



Toggle the visibility by activating . You can also choose one of the other buttons to toggle all child items in the hierarchy or to hide all others.

Visibility of spectra is indicated by a line next to their descriptions. The color of this line is the same as that displayed in the plot.



In order to completely remove a spectrum from the data browser, delete its data first:

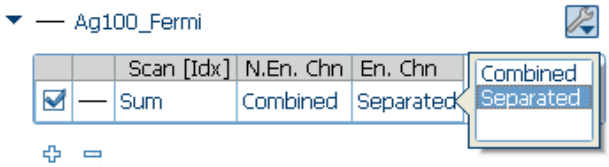
1. Select the spectrum (or spectra) in the Experiment Editor and click . SpecsLab Prodigy will prompt you before the data is deleted.
2. Click the icon to remove the definition of the spectrum from the group.

4.2 Displaying Spectrum Components

By default, the total signal intensity is displayed in the Plot View. You can change the display so that individual channels become visible (for multichannel detectors) or individual scans are shown (when multiple passes are scanned in the spectrum). Other scanning options, such as depth profiling, contain additional components that can be selected. Clearly, the options available depend on your configuration and experiment type.

As an example, to display individual channels in a spectrum:

- Double-click the *Combined* button under *En. Chn* and select *Separated* from the drop-down list.



You can show the individual channels on the Z-axis:

1. Click the icon in the toolbar.
2. Select *Channels* for the Z axis label.

4.3 Performing Operations on Regions of Interest

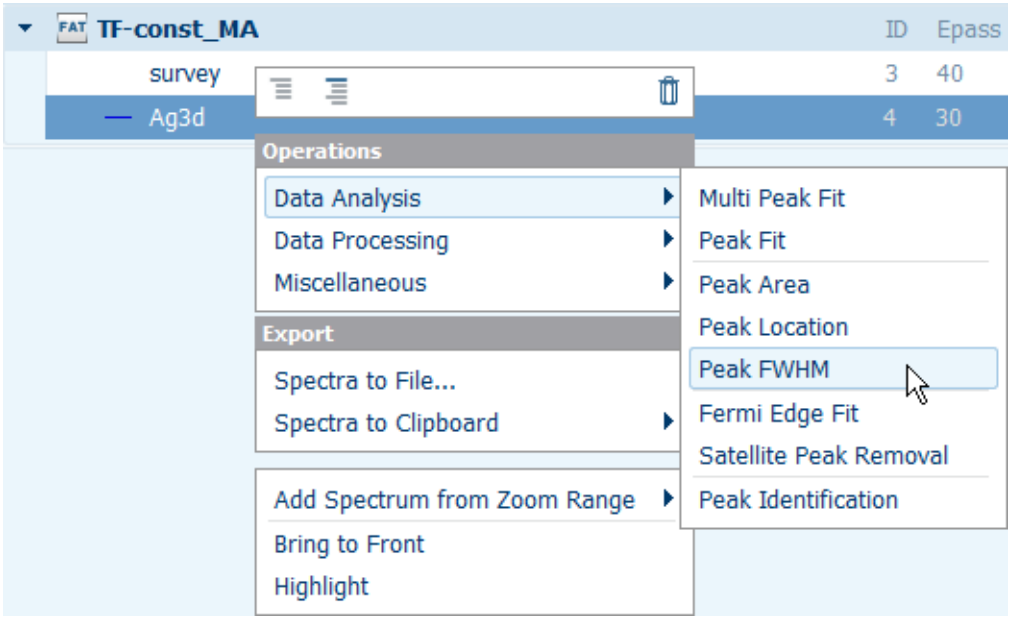
After acquiring a spectrum, you can run data operations on the whole spectrum or on specific regions of interest for data analysis.

Note

If you do not select a region of interest in the following procedure, the data operation will be performed on the whole spectrum.

To perform a data operation:

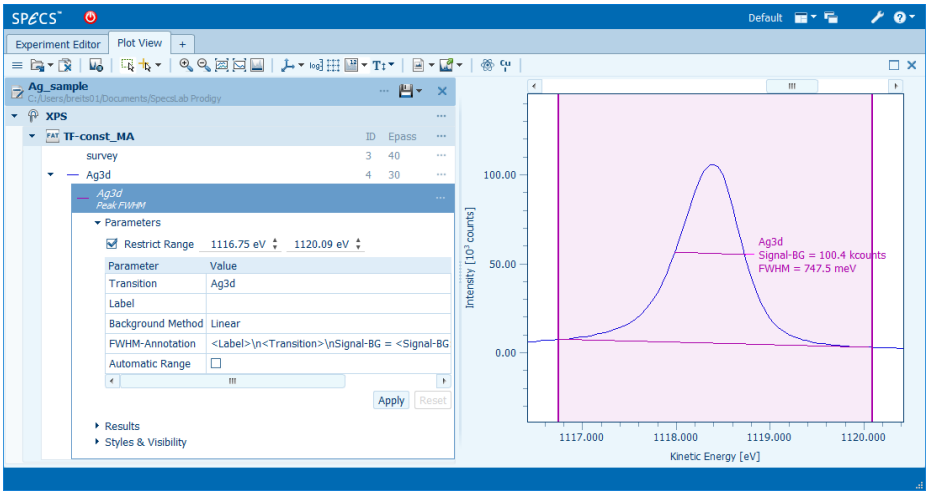
1. Click the icon in the Plot View toolbar.
2. Select a region of interest in the plot. The data operation will be applied to the data in this area.
3. Right-click on the spectrum to be examined. Alternatively, click the icon to the right. A menu with a section *Operations* at the top will appear. Pick, for example, an FWHM calculation from the submenu *Data Analysis*:



After a data operation is specified, it will be performed on the selected region. The operation is displayed in the data browser below the chosen spectrum.

4. Click on the operation to toggle its visibility.

After clicking on it, the operation expands providing access to the input and output parameters, which you may want to alter. Adjust, for example, the range of the calculation, modify labels used in the plot or copy values from the results table:



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