Bruker EMXplus and Xenon Training Manual

Rev 220711

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With Excerpts from the *Bruker Xenon User's Guide*.

Subject **Page Number**

Overview of Operation

The Bruker EMXplus EPR spectrometer is located in GSRC 108H. Its operation is complex and requires significant user interaction. There is very limited automation with the system. The system operates on a Linux workstation running Bruker's Xenon Software. This training guide contains many excerpts from the ***Bruker Xenon User's Guide***. The ***User's Guide*** is very through and well written and is available as a PDF file on the workstation's desktop. We recommend that you read it, especially the sections on theory, instrument description, parameter adjustment and processing results.

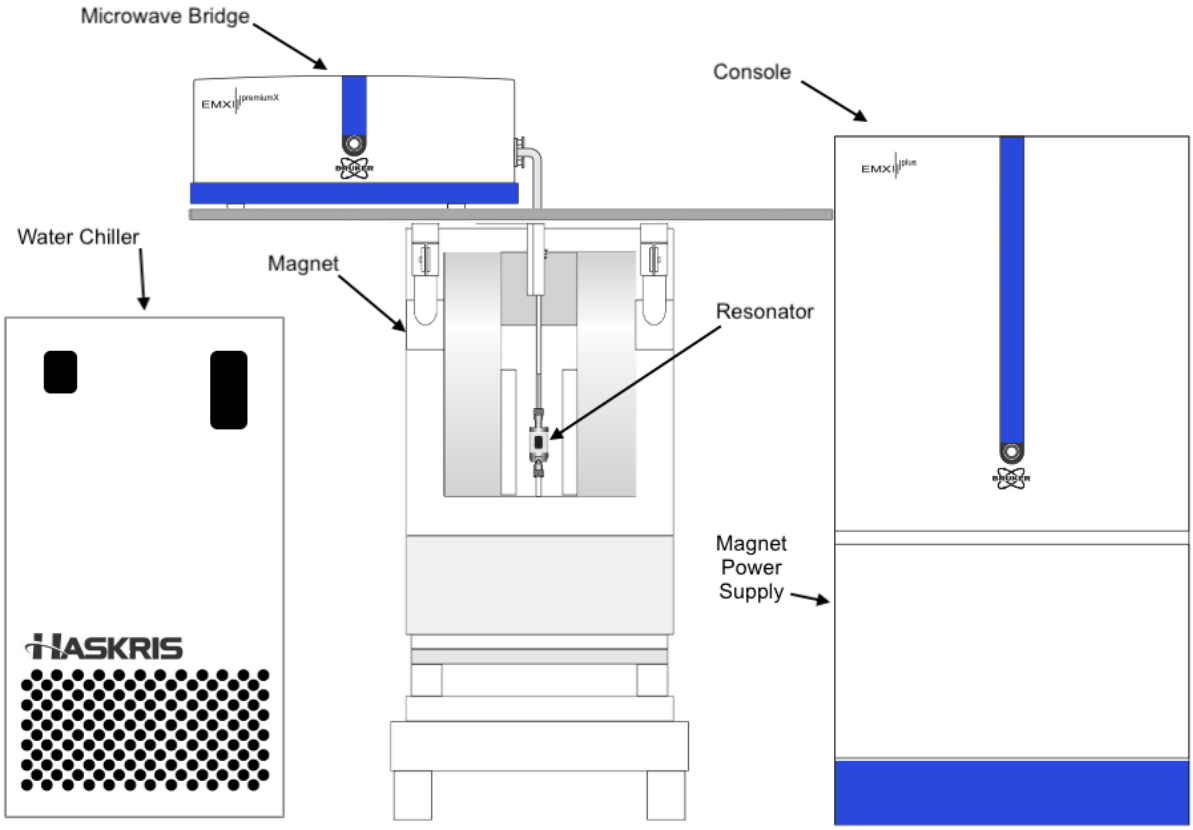
Reading this Guide or the Bruker Manual **are not a replacement for hands on training**. Please contact the staff for scheduling a session.

Here is the usual order of operation with pages in this handout that includes a description.

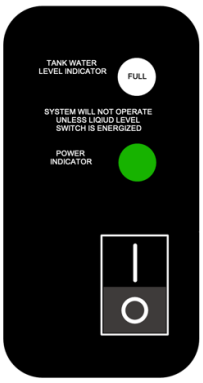
1. Sign into the logbook!
2. Power on instrument (page 2)
3. Connect to instrument in Xenon (page 3)
4. Clean the outside of your sample tube
5. Insert sample into resonator (page 6)
6. Tune the resonator (page 8)
7. Select and optimize acquisition parameters (page 12)
8. Collect spectrum (page 13)
9. View and process the results
10. Save the results (page 25)
11. Optional: Generate an output file (ascii or graphic) (page 26)
12. Remove sample from resonator (page 7)
13. Shut the system off (page 15)
14. Sign out of the logbook.

Turning On the Bruker EMXplus EPR Spectrometer.

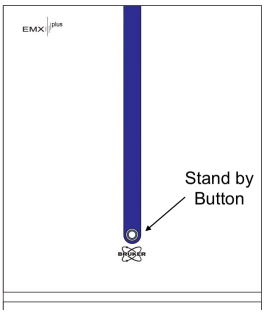
The Bruker EMXplus has six main components that are labeled in the following figure. You should find the console in stand-by mode and the light on the front of the console blinking. The magnet power supply and water chiller should be off. Turn the system on in the following order:



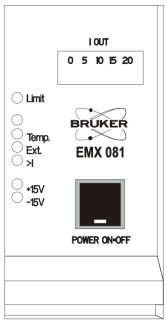
1. Turn on the *Haskris Recirculating Chiller* with the switch in the front of the unit.



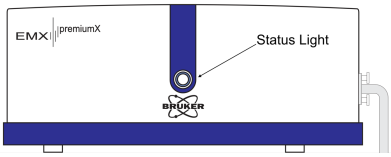
2. Turn on the *Console* by pushing the button on the front door of the console.



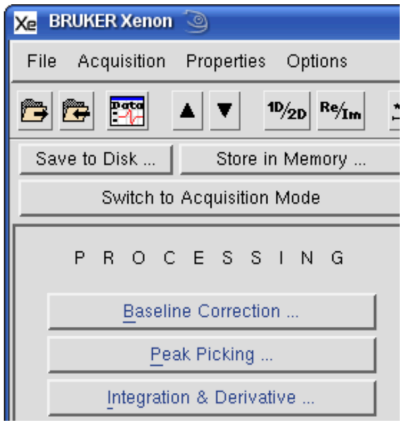
3. Open the door of the *Magnet Power Supply* and turn it on by pushing the power button.

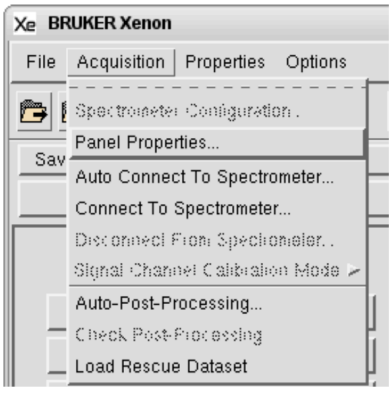


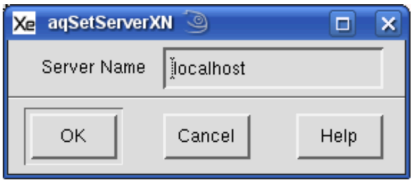
4. The Status Light on the *Microwave Bridge* should start flashing as it initializes. Wait until the light is solid blue before proceeding to connecting the Xenon software that is running on the Linux computer. It will take about 30 seconds for the bridge to be ready.



5. Either find *Xenon* running on the Linux workstation or double click the desktop icon. From the **Acquisition Menu** choose "**Connect to Spectrometer**". When the dialog box opens for the Server name click **OK**.



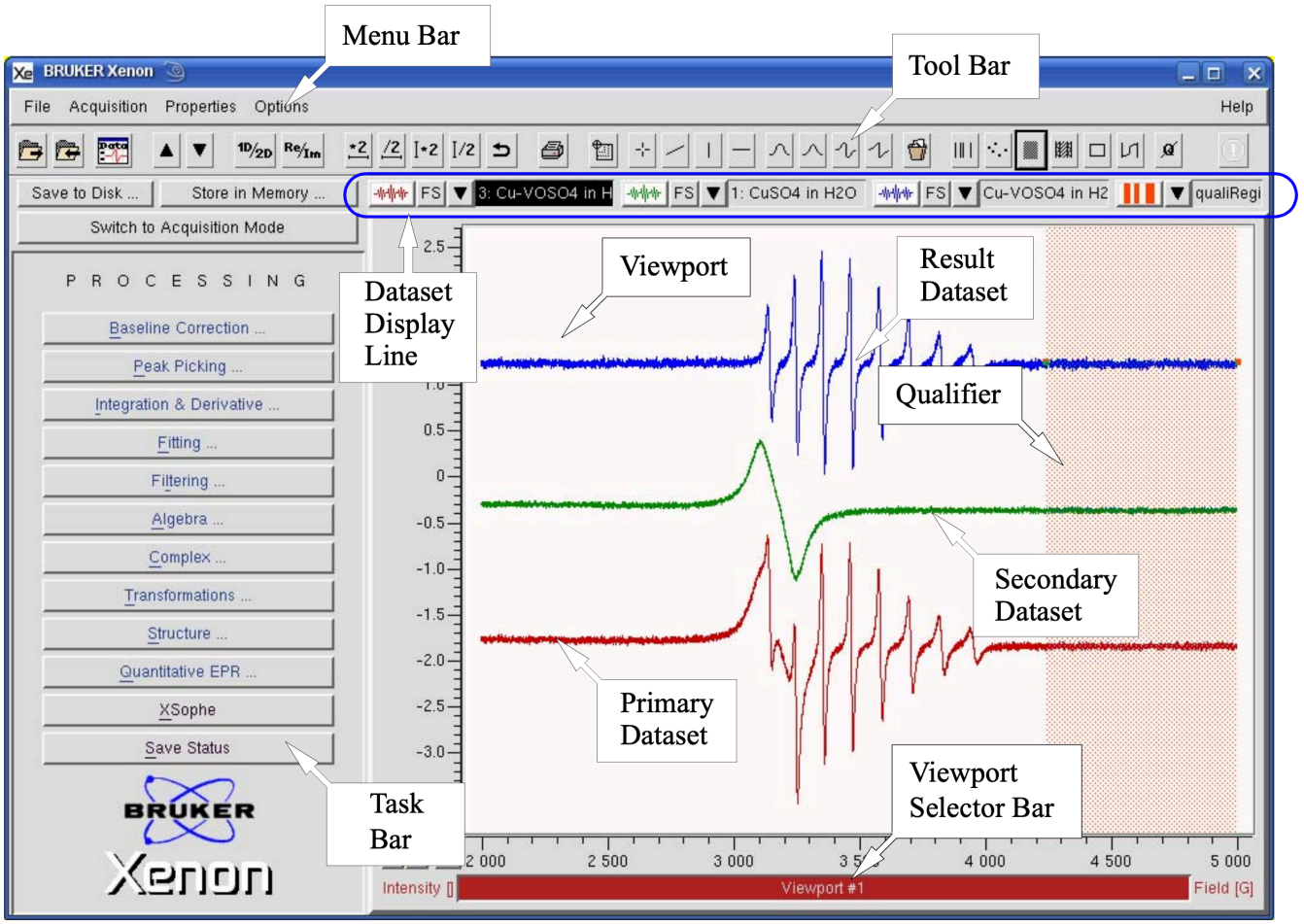




The system should connect within about 30 seconds.

Xenon EPR Software Overview

The EMXplus spectrometer is controlled by a software program called Xenon. This software also includes basic and advanced processing capabilities. An operator can switch between these two operation modes. You should find the program in processing mode and the window will look like the figure below.



The components for the processing mode are:

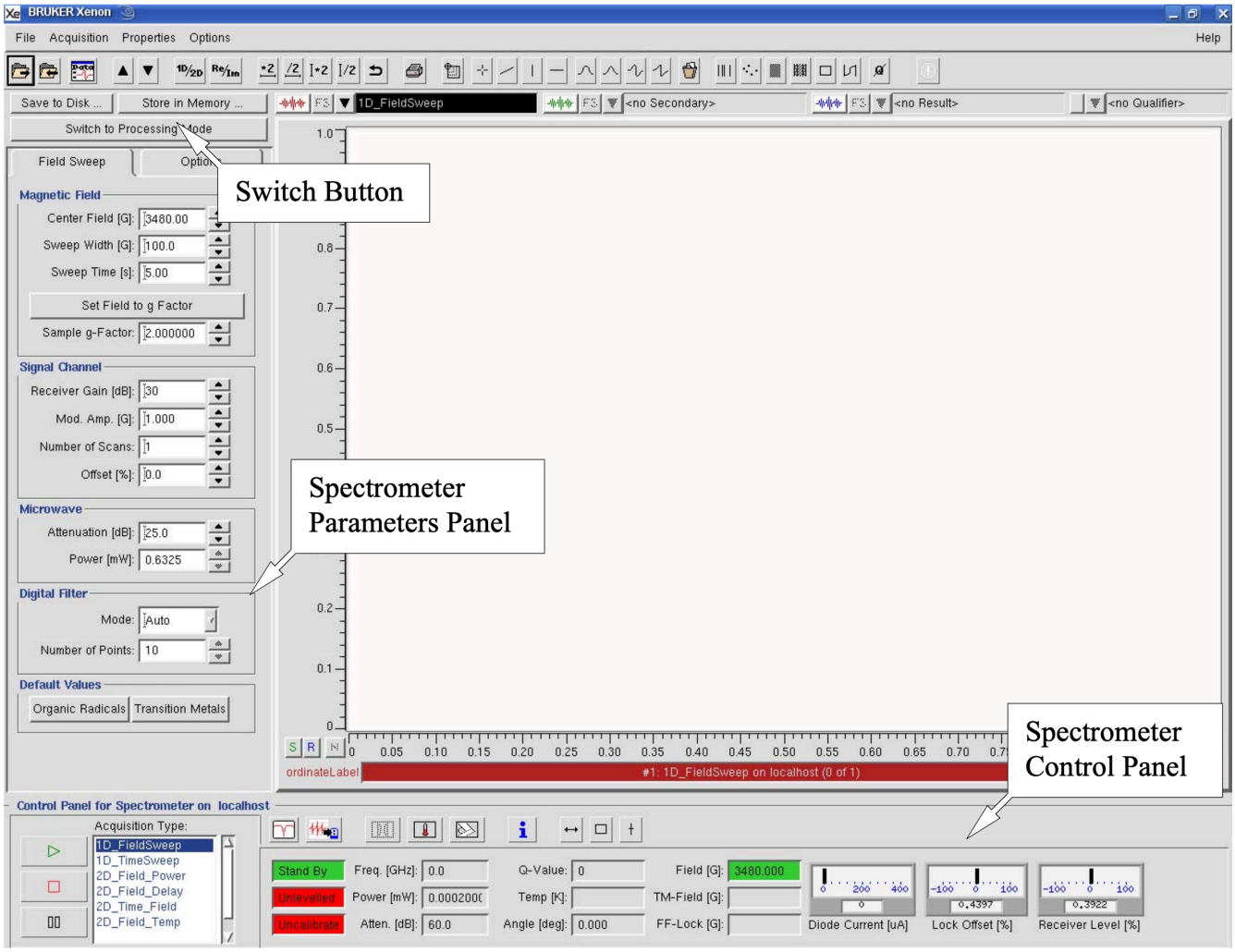
Menu Bar: The menu bar groups several menus together. The File menu deals with input and output of files. The Acquisition menu lets you configure the spectrometer. The Properties menu sets up the Xenon window's features. In the Options menu you can modify the behavior and properties of tools and load external ProDEL programs.

Tool Bar: Buttons for frequently used commands and operations are grouped here for your convenience.

Task Bar: Tasks are macros which organize and streamline the individual processing steps required to perform common operations such as Baseline Correction, Integration, and Peak Picking. These routines are grouped together in the Task Bar.

Viewports: The window in the center is called the Viewport. It displays your data. Please see below and the Bruker Manual for a full description of Viewports, the control buttons and their functions.

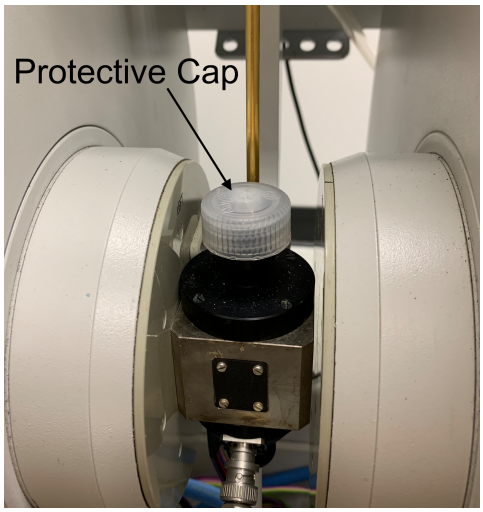
The program window will look different in **Acquisition mode**.



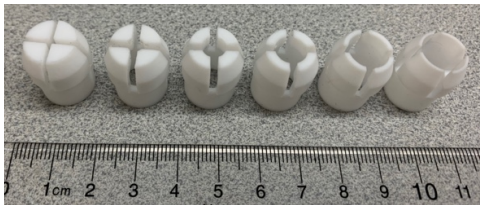
In this mode, the left side of the application window displays the acquisition parameters. The switch button switches between the two modes. It shares many of the same features as the processing mode window but also has a spectrometer control panel for monitoring spectrometer conditions, selecting experiments, and starting, stopping, and pausing experiments.

Inserting and Removing Samples.

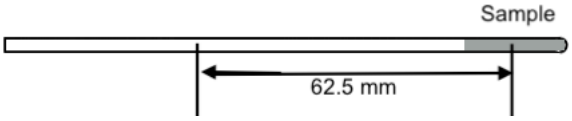
1. If present, remove the protective cap that keeps dust out of the resonator

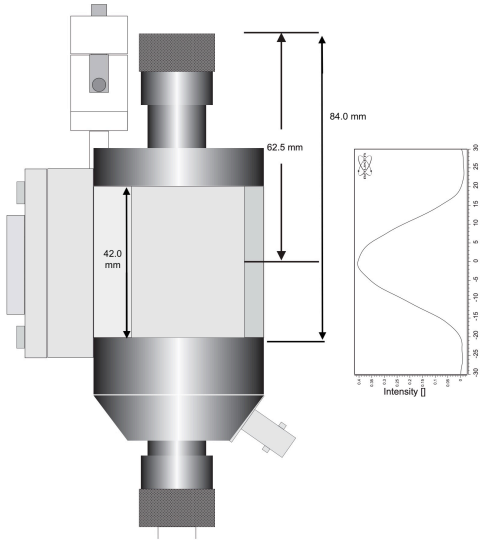


2. Determine the proper collet needed to hold the sample tube. The standard tubes are 4mm o.d. and that collet should be left in the resonator opening. If necessary swap out the collet that fits your sample tube.



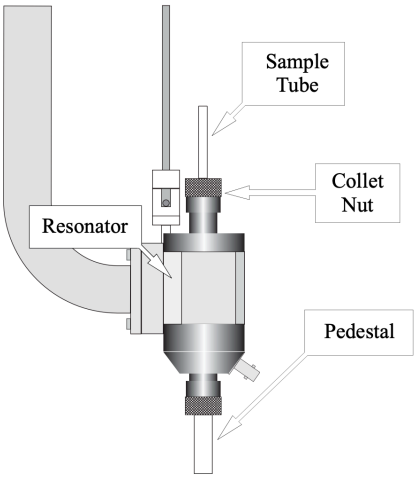
3. Determine the proper depth of your sample. The active height of the resonator is 42 mm. Therefore:
    a. If your sample height is longer than 42 mm; you can place the depth of the tube 84.0 mm from the top collet and the whole length of the resonator would be filled.
    b. If your sample height is less than 42 mm then you need to determine the distance needed to center the sample 62.5 mm from the top collet.





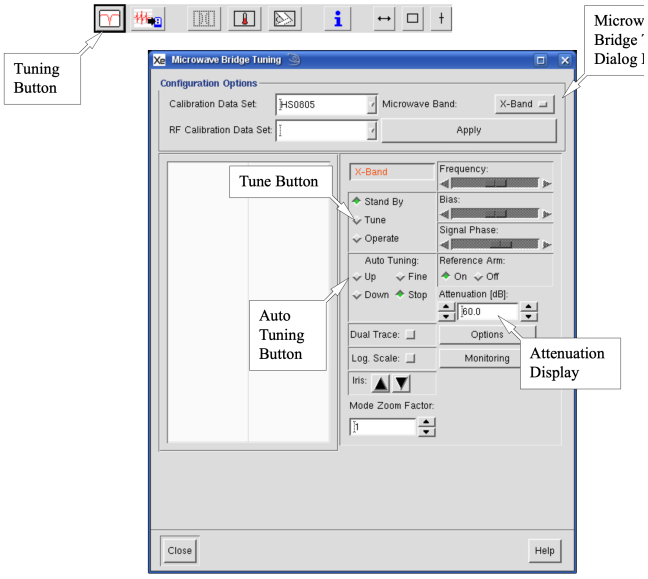
4. Clean the sample tube with a chemwipe. If the tube has visible signs of dirt, clean the tube with some isopropanol that is provided in the lab.

5. Carefully insert the tube into the collet opening. Loosen the collet nut if there is resistance. Push the tube to the depth you determined in step 3. If necessary, loosen the collet nut that holds the pedestal to allow the tube to be fully inserted. Once the tube is at the correct depth, push the pedestal up so that it meets the base of the tube. The sample needs to rest in the indentation of the pedestal so that it is has proper horizontal alignment. Tighten both the pedestal and upper collet nuts so the tube is firmly held in place.



Sample Removal or Exchange

Before removing or exchanging samples you must first open the **Tune Window** and exit out of **Operate** mode. If you are going to run another sample; click on the **Tune button**. If you are going to shut off the instrument, click on the **Stand By button.**



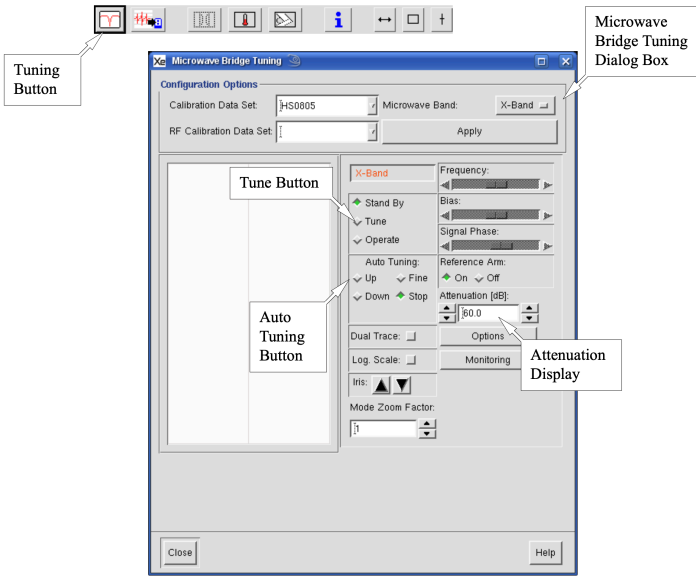
Sample removal is done by loosening the top collect and carefully pulling the tube straight up. If you are exchanging samples of the same height, the pedestal can remain in the same position. Lower the new sample until it meets the indentation of the pedestal for proper alignment before tightening the upper collet nut. If you are finished using the instrument place the protective cap back over the empty resonator opening.

Tuning the Resonator

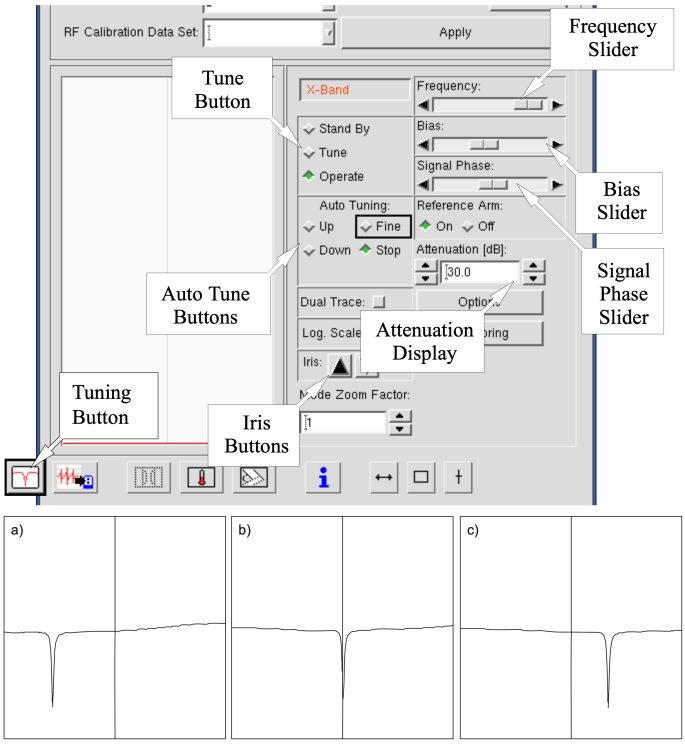
Tuning is the most important step to get consistent and accurate EPR results. It is also the most difficult part of operating the instrument. The auto-tuning can perform very well but often fails, so a user should be prepared to manually tune the resonator. Even with auto-tuning, some prior manual adjustments can greatly increase the success rate. These procedures should work with most solid samples. See the staff if you are having any issues or plan to run liquid or lossy samples.

Preparing for Auto-tuning

1. Open the Microwave Bridge Tuning dialog box. Click the **Tuning button** in the spectrometer control panel.
2. Click the **Tune button** in the dialog box to change to Tune mode.
3. Set the **Microwave Attenuation** to 20 dB. The **Microwave Attenuation** is set by clicking the arrows on either side of the **Attenuation** display in the dialog box. The arrows on the left change the attenuator in 10 dB steps; those on the right in 1 dB steps. You can also click on the number and type in a value.



4. Adjust the **Frequency slider** bar to locate and center the resonator dip in the display monitor. Moving the **Frequency slider** to the right moves the dip to the right and moving it to the left moves the dip to the left. There are three ways to move the slider with varying degrees of fineness. Grabbing and dragging the slider moves the Frequency quickly but very coarsely. This is not recommended since the dip can pass through the window without being seen. Clicking in the white area changes the Frequency in coarse steps. Clicking the arrows on the sides moves the Frequency in the finest steps. Give the system some time to set the frequency after each adjustment.



5. Maximize the depth of the resonator dip by adjusting the Iris. Click and hold either the up or down **Iris button**. This step reduces the amount of microwave power that is reflected back from the resonator. The optimum condition is often called matched or critically coupled. There are two other conditions as well. The undercoupled condition occurs when the iris screw is too high. As you lower the iris screw, critical coupling occurs when the dip is deepest. If you continue to lower the screw, the overcoupled condition occurs and the dip starts to go up again and to broaden.

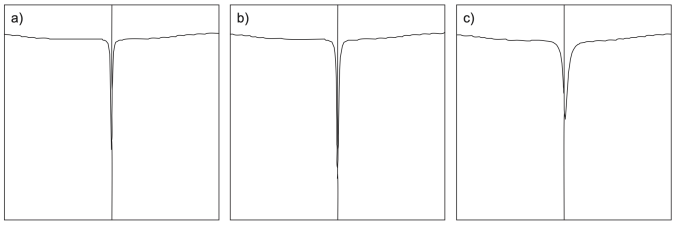
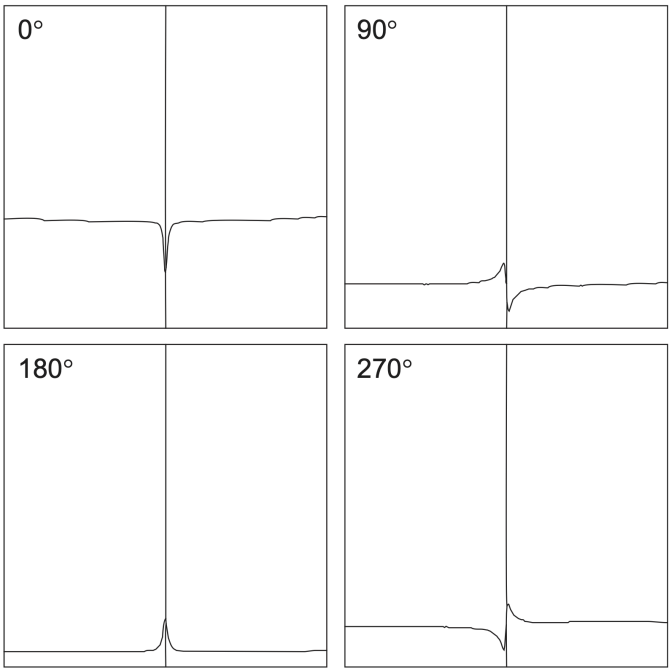


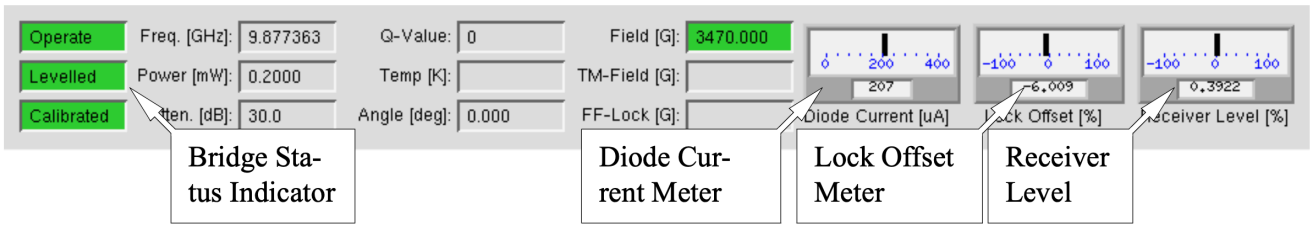
Figure 9-8 Three coupling regimes: a) undercoupled, b) critically coupled, c) overcoupled.

6. If necessary, adjust the **Signal Phase slider** until the dip is negative going and the dip shoulders look somewhat symmetric like the 0° display to the right.



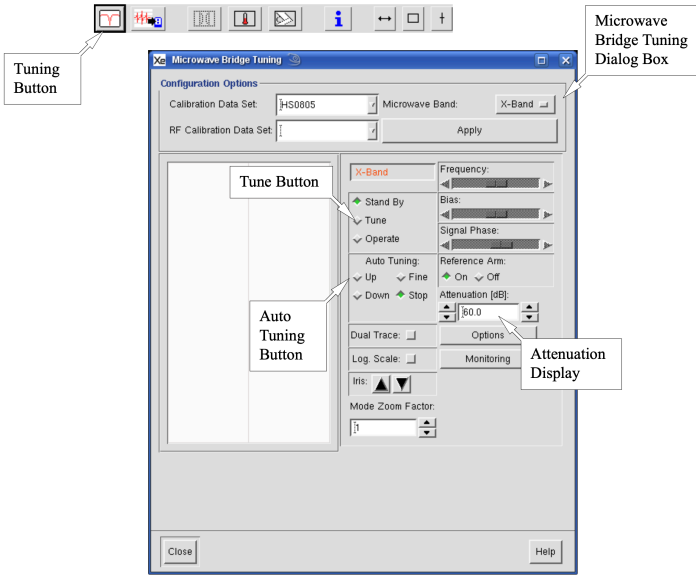
7. Start the Auto-Tune procedure by pressing either the **Up button** or **Down button.** The Up button starts by scanning the microwave frequency up in search of the resonator dip (or frequency where the resonator resonates). The Down button starts by scanning the microwave frequency down in search of the resonator dip. If you are not sure if the search should start up or down, do not worry. The frequency is scanned until its limit is reached and then scan in the other direction until the resonator dip is found. The Auto-Tune routine adjusts the frequency, phase, and bias of the bridge and the coupling (matching) of the resonator. If there is an error message, try repeating this procedure from Step 4. If it fails again you will have to tune manually (see below).

When properly tuned the three indicators on the left side of the Spectrometer control panel should be green and the meters to the right should all be centered. If they drift away from the center, Click on the **Fine Button** in the **Auto-Tuning** section in the Tune dialog box. If that does not work repeat the tuning process.

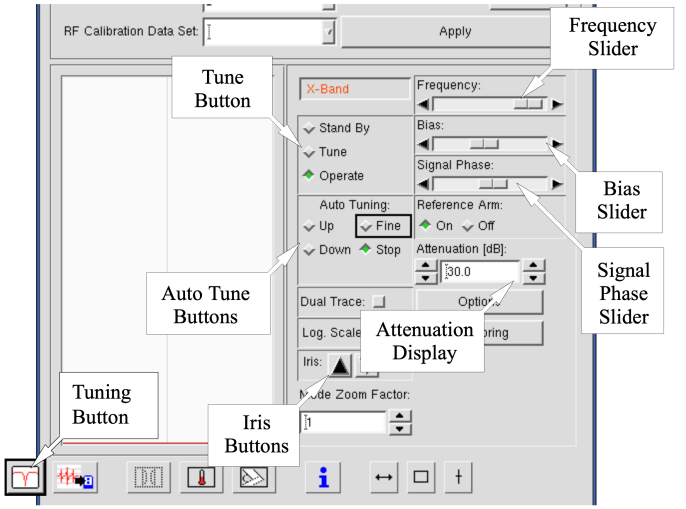


Manually Tuning the Resonator

1. Open the Microwave Bridge Tuning dialog box. Click the **Tuning button** in the spectrometer control panel.
2. Click the **Tune button** in the dialog box to change to Tune mode.
3. Set the **Microwave Attenuation** to 20 dB. The microwave attenuation is set by clicking the arrows on either side of the **Attenuation** display in the dialog box. The arrows on the left change the attenuator in 10 dB steps; those on the right in 1 dB steps. You can also click on the number and type in a value.



4. Adjust the **Frequency slider** bar to locate and center the resonator dip in the display monitor. Moving the **Frequency slider** to the right moves the dip to the right and moving it to the left moves the dip to the left. There are three ways to move the slider with varying degrees of fineness. Grabbing and dragging the slider moves the Frequency quickly but very coarsely. This is not recommended since the dip can pass through the window without being seen. Clicking in the white area changes the Frequency in coarse steps. Clicking the arrows on the sides moves the Frequency in the finest steps. Give the system some time to set the frequency after each adjustment.



5. Maximize the depth of the resonator dip by adjusting the Iris. Click and hold either the up or down **Iris button**. This step reduces the amount of microwave power that is reflected back from the resonator. The optimum condition is often called matched or critically coupled. There are two other conditions as well. The undercoupled condition occurs when the iris screw is too high. As you lower the iris screw,

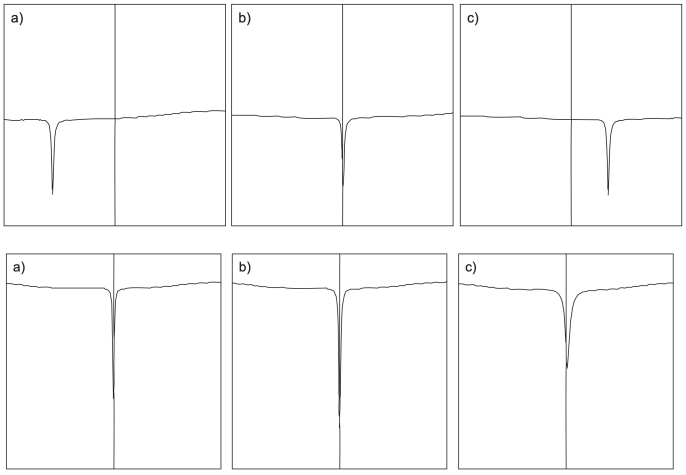
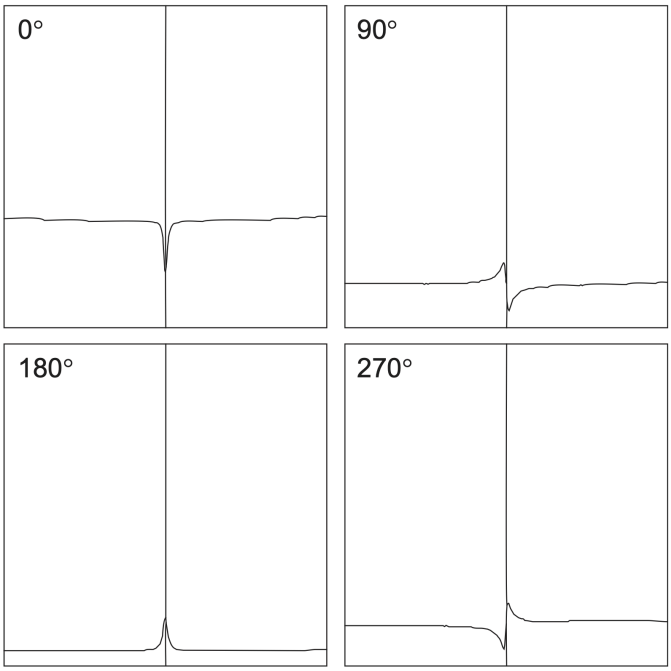


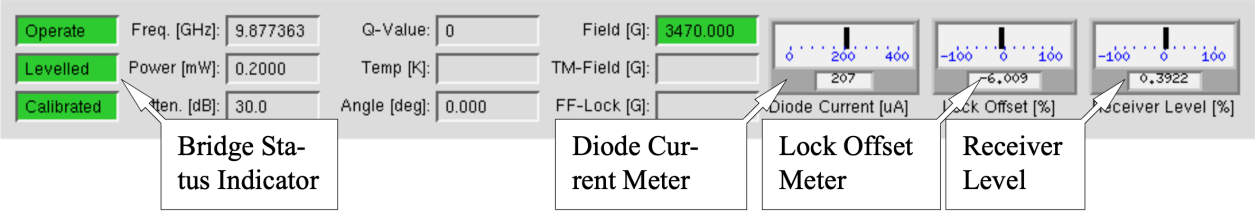
Figure 9-8 Three coupling regimes: a) undercoupled, b) critically coupled, c) overcoupled.

critical coupling occurs when the dip is deepest. If you continue to lower the screw, the overcoupled condition occurs and the dip starts to go up again and to broaden.



6. If necessary, adjust the **Signal Phase slider** until the dip is negative going and the dip shoulders look somewhat symmetric like the 0° display to the right.

7. Click on the **Operate Button** in the Tune Dialog Window and change the microwave attenuation to 60 dB. Then focus your attention on the Diode Current meter in the Spectrometer control panel.



Use the **Bias Slider** in the Tune Dialog Window to set the Diode Current to the center (200 μA). Only adjust the **Bias** when the attenuation is 50 db or higher.

8. Change the microwave attenuation to 50 dB. If the Diode Current increases, adjust the **Irix down** until the current is centered in the meter. (If the current meter is below 200 μA move the Iris up.) If the Lock offset Meter is not at the center (0%), adjust the **Frequency slider** with the fine controls to recenter. Move the **Frequency slider** in the direction you want the meter to go.
9. Change the microwave attenuation to 40 dB and repeat the optimization in step 8.
10. Change the microwave attenuation to 30 dB and repeat the optimization in step 8.
11. Change the microwave attenuation to 20 dB and repeat the optimization in step 8.
12. Maximize the Diode current with fine adjustments of the **Phase Slider.** Adjust the **Iris down** if the Diode current increases above the center and adjust the **Frequency** to center the Lock offset if it moves from the center.

When properly tuned the three indicators on the left side of the Spectrometer control panel should be green and the meters to the right should all be centered. If they drift away from the center, Click on the **Fine Button** in the **Auto-Tuning** section in the Tune dialog box. If that does not work repeat the manual tuning process.

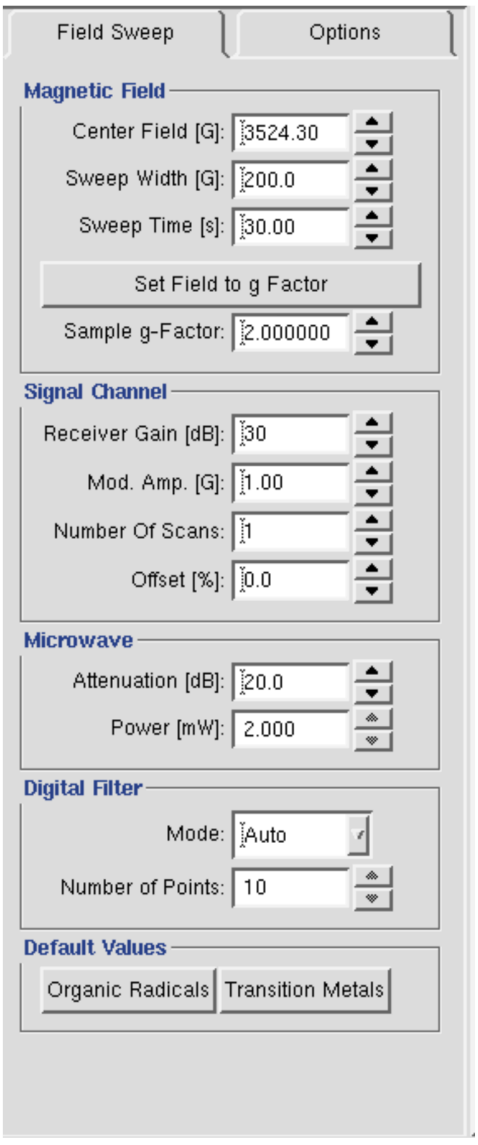
Basic Data Collection in Xenon:

Once the sample is inserted and the resonator is tuned, data can be collected. Xenon offers two basic parameter sets to start your experiment setup. They can be loaded with the buttons on the bottom of the left-hand **Parameter Panel** under the **Field Tab**. The choices are:

Organic Radicals: Narrow field sweep around g = 2. Appropriate for most non-metal centered radicals.

Transition Metals: Large field sweep to cover the range of most metal centered radicals.

The Bruker manual has an excellent description of the parameters and how to optimize them. This training note will highlight some of the important parameters you should consider when running your samples. The parameters below are the starting point for the ***Organic Radicals*** parameters. See the manual for the changes with the ***Transition Metals*** parameters.



The Field Sweep Tab

The Magnetic field defaults are a good place to start. You can narrow the ***Sweep Width*** to save time and you can increase the ***Sweep Time*** to improve resolution.

The ***Receiver Gain*** setting is not changed when you load either default starting parameters. 30 dB is a good starting point. If you see peak tops clipped; lower the gain. Increase if signal is weak.

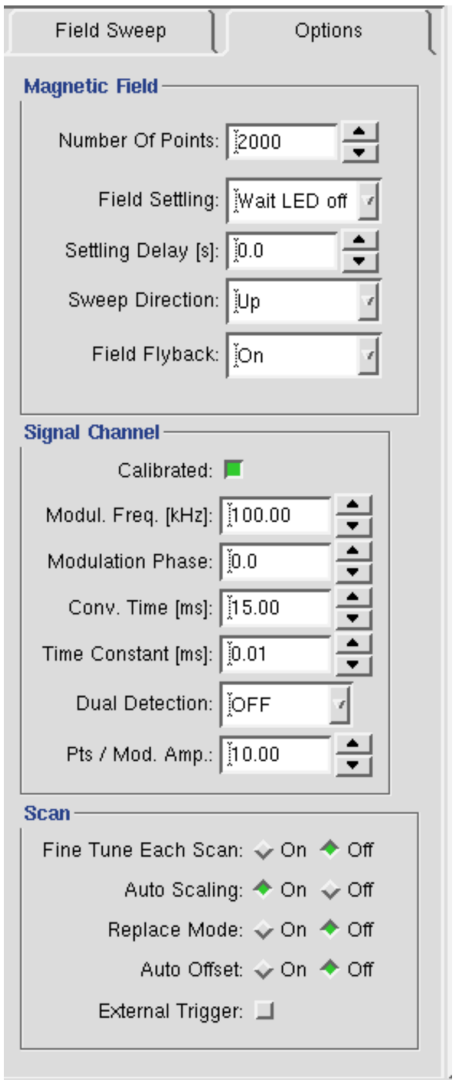
The ***Modulation Amplitude*** is one of the more important parameters. Too large and you get line broadening and distortion. Too small and the sensitivity can be poor. If you expect sharp lines leave this set to 1 G. Increase this up to the line width (2-5 G) to improve sensitivity on broader peaks.

Signal to noise can also be increased by running multiple scans.

2mW of Microwave ***Power*** should be adequate for most samples. Leave attenuation set to 20 dB. Increase attenuation *(i.e., lower power)* if peaks are saturated.

If possible, we recommend turning off the **Digital Filter** and smoothing the spectrum in processing mode. Digital filtering here is irreversible, while smoothing after collection can be optimized in a reversible fashion. To turn off Digital filtering set the ***Mode*** to "Manual" and the ***Number of Points*** to "1".

The buttons to load the Default parameter Values



The Options Tab

The ***Number of Points***, the ***Conversion time*** and the ***Modulation Frequency*** have a connected relationship. You cannot set the ***Number of Points*** directly and it could be a very low number by default. A desired value is close to 1000 and is adjusted by changing the ***Point per Modulation Amplitude*** below.

The ***Field Settling*** is important for experiments collecting multiple scans. The ***Settling Delay*** in combination with ***Field Settling*** set to "Wait Given Delay" can assure each scan starts at the correct field. Setting ***Field Settling*** to "Wait Stable" usually will give good results with multiple scans with minimal wait between scans.

A ***Modulation Frequency*** of 100 kHz will be adequate for most experiments.

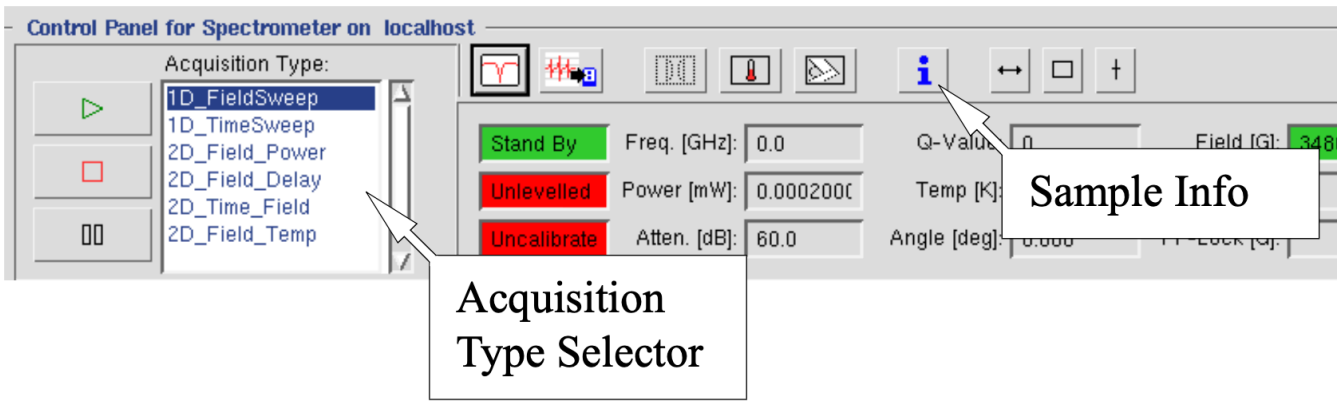
The ***Conversion Time*** is the time spent at each point and should be left unchanged.

The ***Time Constant*** is an analog filter setting to help signal to noise. Increasing this value will reduce noise however you can lose fine structure and peak intensity. A safe rule of thumb is to keep the ***Time Constant*** much less than the ***Conversion Time*** (≤10%).

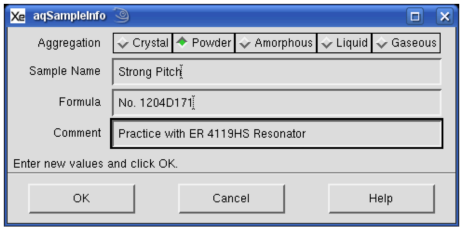
The ***Points per Modulation Amplitude*** will control the number of points collected. Set this so the ***Number of Points*** is between 1000 -1200.

The ***Fine Tune Each Scan*** is very helpful for large number of scans (long acquisition). It will allow the instrument to touch up the cavity tuning to compensate for any instrument drift that occurs during the experiment.

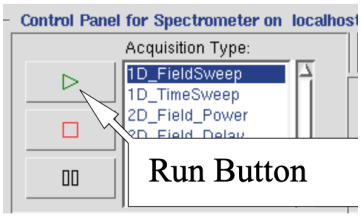
The system has several Acquisition Types. Check that the **1D_FieldSweep** is chosen in the Spectrometer Control Panel. It is good practice to enter Sample Information that will be saved and printed with the results.



The Sample Information Dialog box that opens when you select the **Sample Information button**.



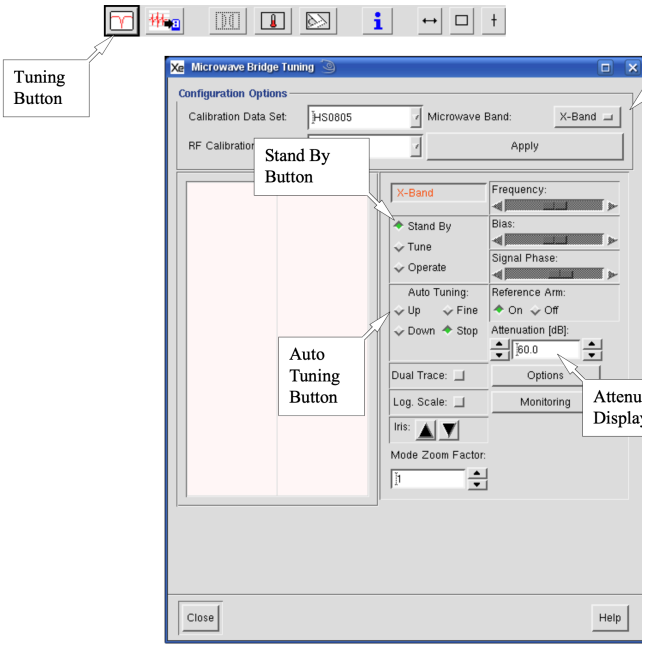
Collect Data by clicking on the **Run button**. You can abort a run with the **Stop Button** or pause a run with the **Pause Button**. The current scan will finish before a stop or pause is executed. The spectrum should show in the Viewport as it is scanned.



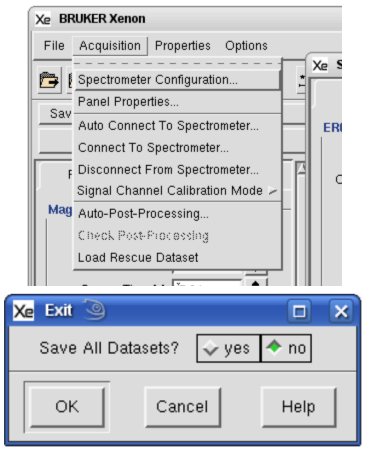
Turning off the System

1. In *Xenon* open the **Tune window** and turn the bridge into **Stand By mode**.

2. Close the **Tune window** by clicking the **Close** button.

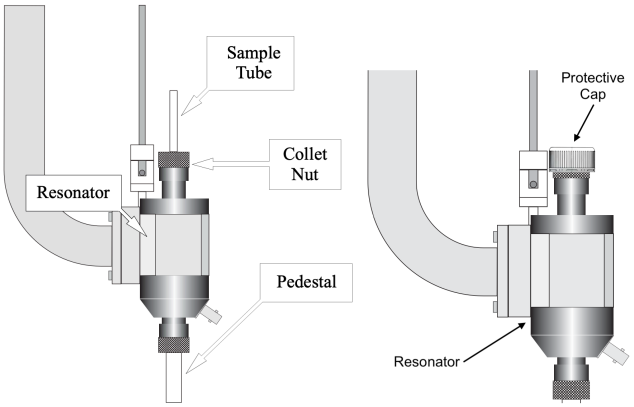


3. In the *Xenon* **Acquisition Menu** choose "**Disconnect from Spectrometer**". A dialog box will open. Select yes or no and then click **OK.** (If you chose yes, then you will need to complete the save dialog)



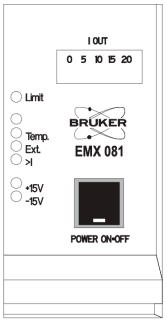
4. Loosen the top collet nut and carefully remove your sample.

5. Cover the cavity opening with the cap.

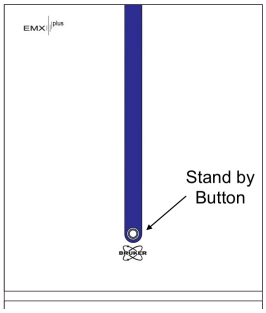


6. Power off the system in the reverse order you performed from power up:

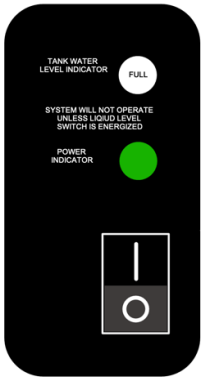
   a. Switch off the *Magnet Power Supply*



   b. Switch the *Console* into Stand By with the button in front.

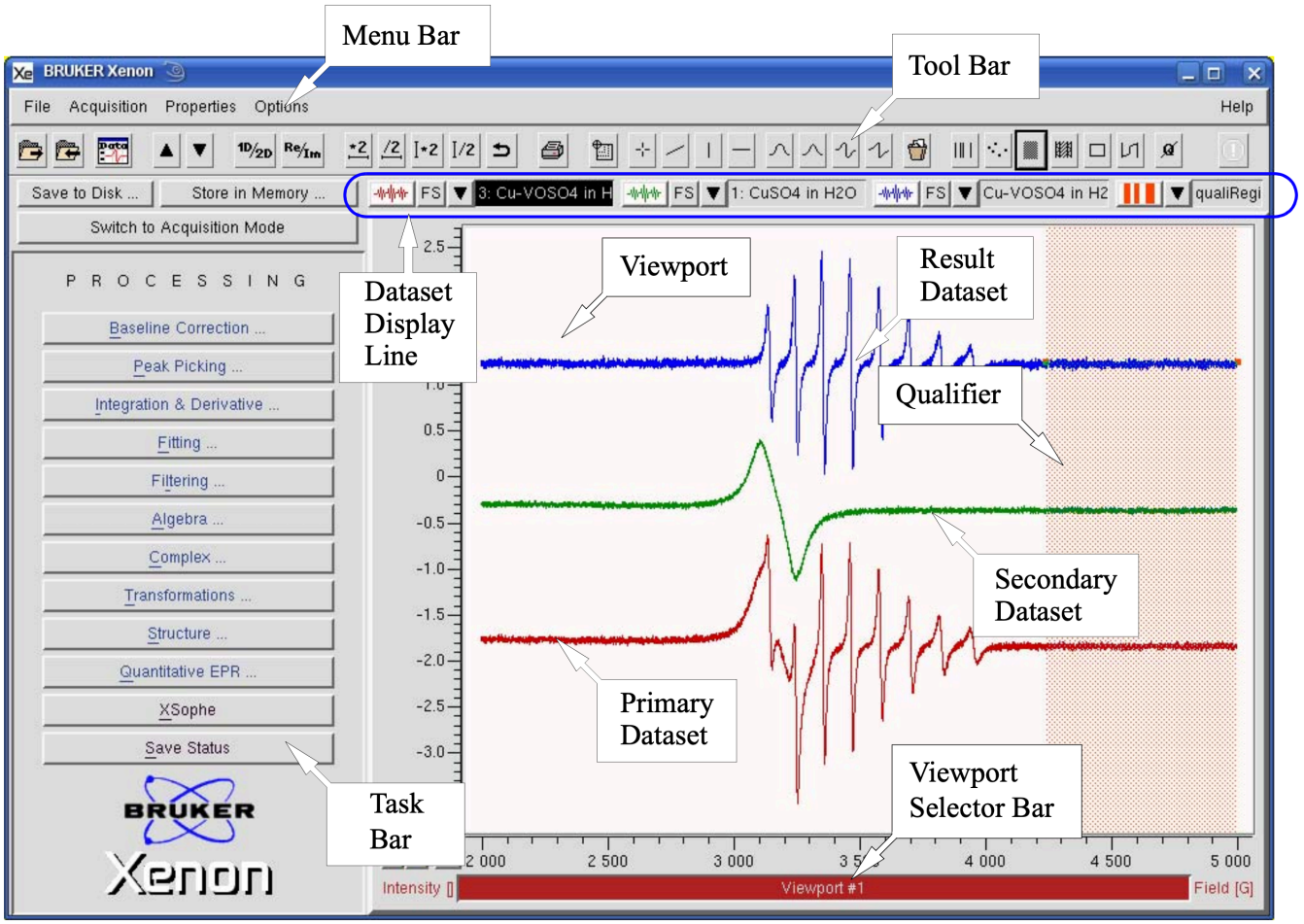


   c. Turn off the *Haskris Chiller* with the switch on its front.



We usually leave Xenon running on the workstation and the user account logged in. Do not forget to log out of the logbook.

Viewing Results in Xenon.



Spectra will be displayed in the Viewport region of Xenon. They can be manipulated and processed with interactive commands accessed from the left had panel called the Task Bar. The Bruker manual has detailed instructions. Some of the more important functions are **Baseline Correction**, **Peak Picking**, Noise smoothing in the **Filtering** option, and **Quantitative EPR**. Please review these topics in the Bruker Manual and see the Staff for additional help.

Viewports

The viewport is the central feature of the Xenon software. All datasets are presented and processed in a viewport. A viewport can show 1D or 2D datasets in the display area with a multitude of options. You can control which datasets are displayed and their options with the Dataset Display Line. When you have more than one spectrum in the viewport, they can be individual scaled by using the individual scale buttons.

Display Area

The center part of a viewport is the display area. By default, the background is white.

Viewport Selector Bar There may be some instances when there is more than one viewport. A red or highlighted bar indicates the active viewport. You can switch active viewports by clicking this bar. It is also used sometimes to display readout information.

There are four types of datasets that can be displayed:

Primary If you only have one dataset, it is normally in the Primary dataset. This is the spectrum which you process or analyze. Its default display color is red.

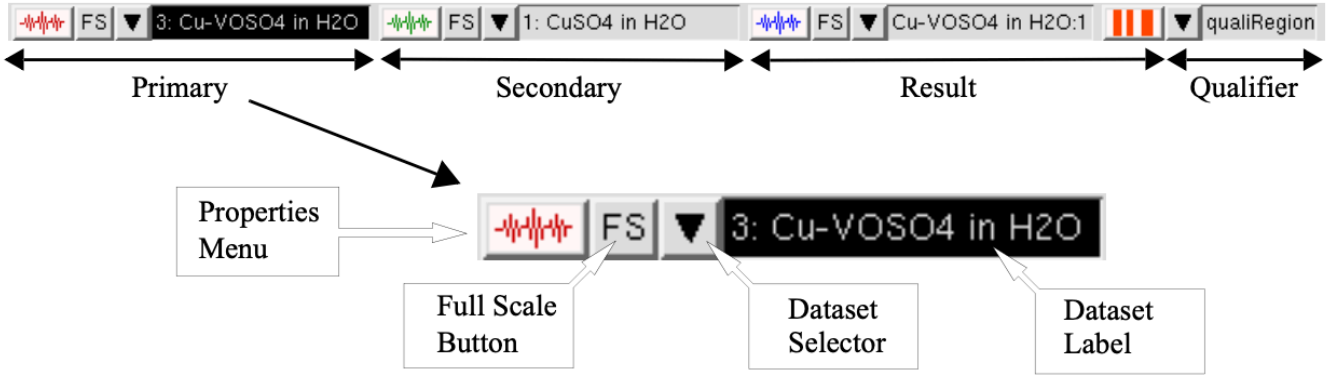
Result After you process the dataset in Primary, the results of your operation are temporarily stored in the Result dataset. The Result and Primary datasets appear simultaneously in the Viewport. Its default display color is blue.

Secondary Some operations require two datasets, such as subtracting two spectra from one another. In this case, the second spectrum should be loaded into the Secondary dataset. Its default display color is green.

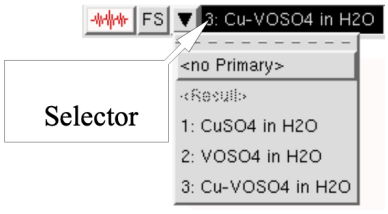
Qualifier The qualifier allows you to define or qualify the region of a dataset which is affected when you perform an operation. By default, the whole dataset is qualified. Its default display color is orange.

Dataset Display Line

Below the tool bar is the **Dataset Display Line**. It is separated into four sections corresponding to the dataset which it controls. Most of the sections consist of four elements which are described below.



Dataset Selector

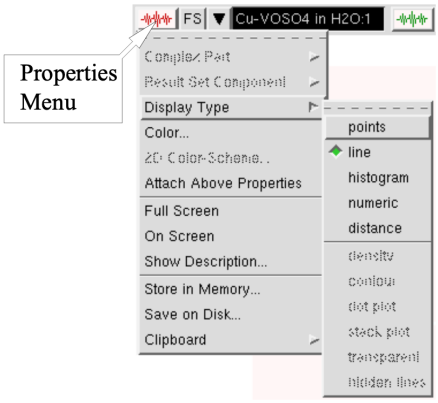


In order to select a dataset, click the small triangle next to the Dataset Label. A menu drops down listing all the datasets that are currently loaded in Xenon. To select the dataset to display in the viewport, click the desired dataset. You can also choose not to show any dataset by clicking <no Primary> (or <no Secondary>...). A particularly useful feature is <Result>. When you click it, it loads the latest Result dataset.

Full Scale Button 

To the left of the Dataset Selector is a button labeled FS. When clicked, it resizes the spectrum so that it completely fills the viewport.

Properties Menu



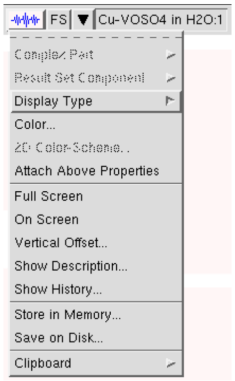
The **Properties** menu allows you to choose the **Display Type**. 1D datasets can be presented as points, line, histogram, numeric, or distance. For 2D datasets you can choose from density, contour, dot plot, stackplot, transparent, and hidden lines.

Show Description allows you to view the parameters of the dataset you select.

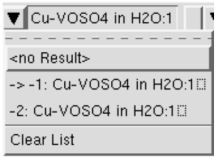
You can store or save the currently displayed dataset. **Store in Memory** temporally saves the data in the memory. When you quit Xenon the data is lost. The **Save on Disk** function writes the data onto the hard disk and makes the data permanent.

The Result Section

The Result section is similar in structure to the Primary section. In the property menu most of the submenus are the same except that there is Show History to allow you to view the data processing history. The FS button is the same. The select menu is a little different. The menu lists the results of each dataset processing operation. It has a <no Result> button to clear the Result from the viewport.



Sometimes when much data is processed the huge amount of data could over- load the memory and slow down the computer. The Clear List button removes all the temporary result data. Store or Save the useful results and use Clear List frequently when you process data intensively.



Individual Scale Buttons

The Individual Scale buttons are found in the lower left part of the Viewport. With them you can set different scales for the Primary, Secondary, and Result datasets. Clicking **S** adjusts the scale for the Secondary dataset only. Clicking **R** allows you to independently adjust the Result dataset scale. An * appears next to S or R when the Secondary or Result dataset scales are different. Clicking **N** brings them back to the same scale as the Primary.

The Tool Bar Functions:

Load Dataset Clicking this button opens a dialog box for choosing the dataset (and its path) you want to load into Xenon.

Save Dataset Clicking this button opens the save file dialog box so that you can save the dataset onto the hard drive. On top, you can select the source (*e.g.* Primary, Secondary, ...) as well as enter a title for the dataset.

Dataset Table This dataset table lists all the datasets loaded or currently stored in memory.

Previous/Next Dataset Clicking this button displays the dataset listed before/after the current dataset in the dataset table.

Toggle Dimension Clicking this button toggles the current active viewport between 1D and 2D views.

Toggle Complex Part Clicking this button toggles the current display between the real and imaginary part of the dataset if the dataset is a complex datset.

X-Range * 2 This button expands the X-axis by a factor of 2.

X-Range / 2 This button shrinks the X-axis by a factor of 2.

Y-Range * 2 This button expands the Y-axis by a factor of 2.

Y-Range / 2 This button shrinks the Y-axis by a factor of 2.

Previous Range Clicking this button brings you back to the previous range.

Print Viewport Click this button to print the spectra in the currently active viewport.

Expand With this button selected you can select regions to zoom or expand with the mouse.

Dot Marker A point marker appears in the current viewport when you click this button. You can use the mouse to move it to where you want. The x and y coordinates are displayed next to the marker.

Free Line This marker provides you with a straight line of arbitrary angle and length. Both ends can be moved by dragging with the mouse. While active, the height and width of the line are displayed in the viewport selector bar.

Free Line This marker provides you with a straight line of arbitrary angle and length. Both ends can be moved by dragging with the mouse. While active, the height and width of the line are displayed in the viewport selector bar.

Horizontal Line This tool is similar to the vertical line except that it is horizontal. While active, the width of the line is displayed in the viewport selector bar.

Gaussian This tool provides you with a gaussian lineshape. You can change its height and width by dragging its handles. While active, the amplitude and full width at half height are displayed in the viewport selector bar.

Lorentzian This tool is similar to the gaussian lineshape except that it is a lorentzian lineshape. While active, the amplitude and full width at half height are displayed in the viewport selector bar.

Derivative Gaussian This tool provides you with a first derivative gaussian lineshape. You can change the height and width with the mouse. While active, the peak-peak amplitude and width are displayed in the viewport selector bar.

Derivative Lorentzian This tool is similar to the derivative gaussian tool except that it is a first derivative lorentzian lineshape. While active, the peak-peak amplitude and width are displayed in the viewport selector bar.

Remove Tool If you use the mouse to select the marker and then click this remove tool button the marker disappears.

Position Qualifier This qualifier provides you with a vertical line and allows you to select an x-axis position for processing. You can drag the qualifier to the exact position you want to select. Once selected, the position qualifier cannot be moved. It can be removed by left-clicking it.

Point Qualifier You can select a point for processing with this tool. Using the mouse, you can precisely move the qualifier to the desired point. Once selected, the point qualifier cannot be moved. It can be removed by left-clicking it.

Region Qualifier Using this qualifier you can select a region of the x-axis for processing. Grabbing the handles on each side, you can move the region to cover the part of the dataset you want to process.

Background Qualifier Using this qualifier you can select a region of the x-axis for background or baseline fitting. Grabbing the handles on each side, you can move the region to cover the part of the dataset you want to fit.

Area Qualifier This tool provides you with a rectangle to cover the area you wish to process. Dragging each corner can change the size of the square.

Integral Qualifier This tool consists of two vertical lines and a free line. The vertical lines indicate the starting and ending points respectively. The free line indicates the offset and the slope. It is designed for integration.

No Qualifier This tool removes the qualifier.

Terminate operation This button stops a process or operation that is running.

Mouse Functions

Depending on which buttons you pressed, the mouse performs many different functions such as resizing, moving, and measuring. By default, the mouse is in auto select mode and changes its function and mouse cursor according to the buttons pressed and location of the cursor. The following examples illustrate the various mouse functions.

The Cursors

The mouse cursor indicates the current mouse function in Xenon.

Expand: When this cursor is present you can click the left mouse button on the position you want to expand and drag the mouse to the place you want to end. A rectangle shows up indicating the area you want to expand. The area covered by the square expands to fill the screen of the viewport.

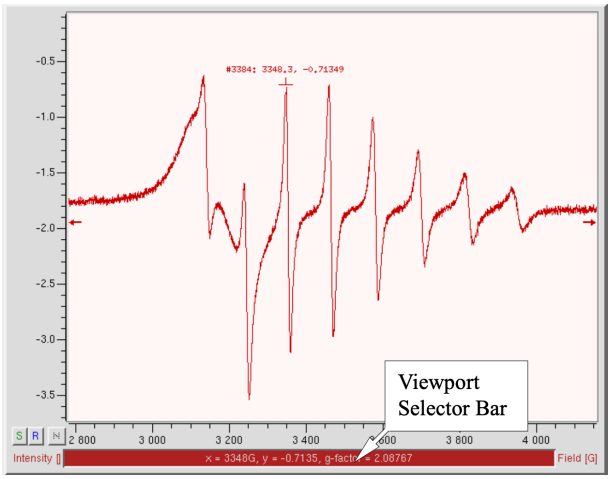
Zoom: This symbol indicates that the zooming function is activated. Clicking with the right mouse button in the display area of the viewport displays this symbol. Dragging the cursor upwards or downwards vertically zooms in or out the area you point to. Dragging towards the right or left horizontally zooms in or out the area you point to. Dragging at an arbitrary angle zooms both horizontally and vertically at the same time. If you click the right mouse button in the x- or y-axis area, you zoom either horizontally or vertically.

Moving: Clicking on the middle mouse button changes the cursor to this symbol. The spectrum moves in the direction you drag the mouse. When you click the middle mouse button in the axis area you only move the spectrum either up and down or to the left and right.

Read Out: With this mouse function you can read out the X-, Y-, and other values of the point where the mouse is in the spectrum. See the next section for details.

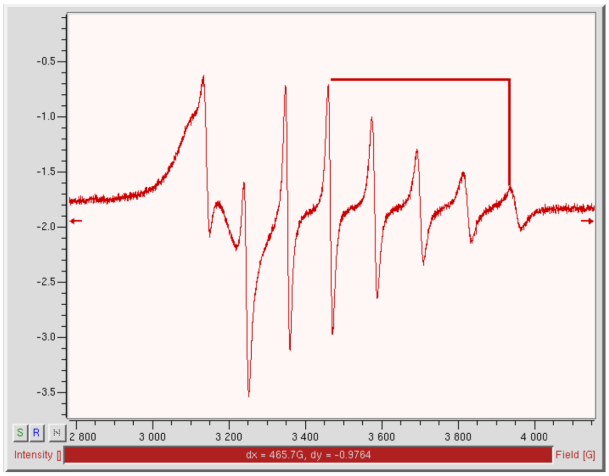
Reading Out Coordinates

Move the mouse cursor close to the spectrum curve. The mouse cursor changes from the Expand to the Read Out cursor. Left click on a point of the spectrum: the coordinates of the cursor are displayed next to the cursor. The field value, intensity, and the g factor value are also displayed inside the Viewport Selector Bar if the spectrum is an EPR field sweep spectrum.



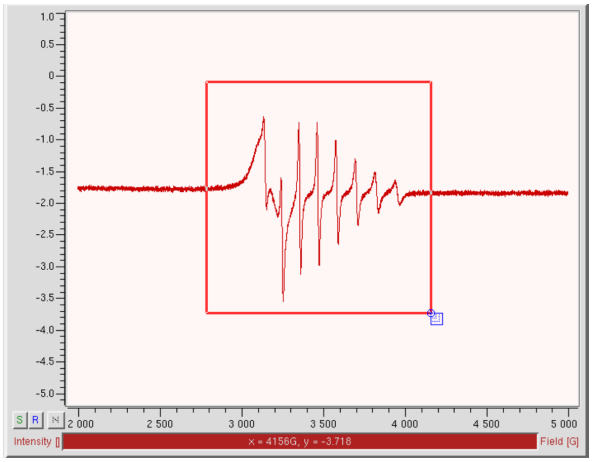
Measuring Distances

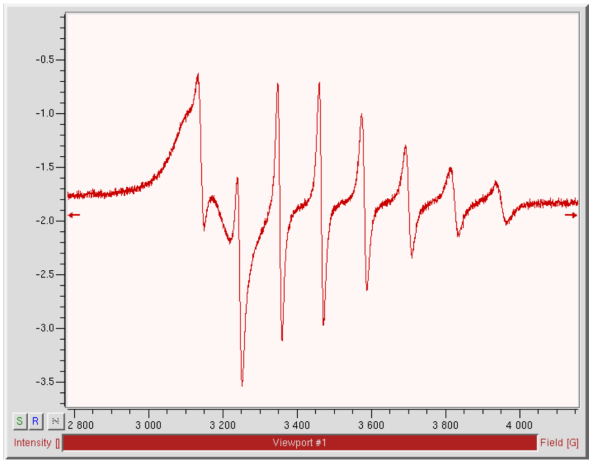
Move the mouse cursor to the starting point. Press the left button and the right button simultaneously. Hold the mouse buttons and drag the cursor to the point where you want to end the measurement. The distance between the starting point and the ending points along the x and y axes are displayed in the Viewport Selector Bar.



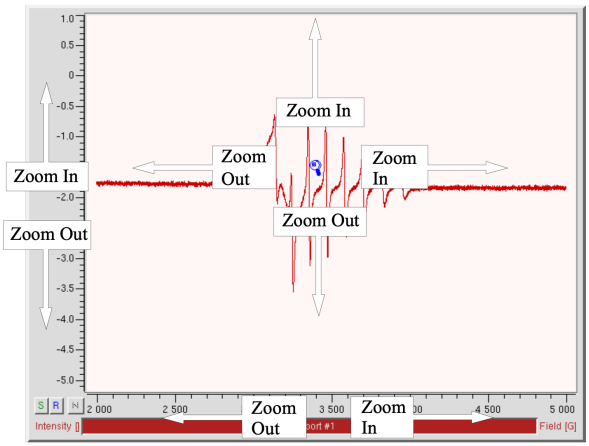
Zooming Spectra

You can zoom in on a specific area of a spectrum by using the rectangular scaling option. Move the mouse pointer to the display area of the viewport. The mouse pointer changes to the expand cursor. Click the left mouse button and drag the rectangle until it encompasses the region of interest. Release the mouse button and the region of interest then expands to fill the viewport.

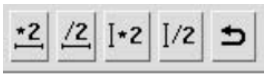




A second means of zooming not only allows you to zoom in but also to zoom out. Place the mouse pointer in the spectrum area or in the axes area where you want to zoom. Click the right mouse button. The mouse pointer changes into a zoom cursor. Dragging up or right zooms in the spectrum or axis. Dragging down or left zooms out the spectrum or axis.

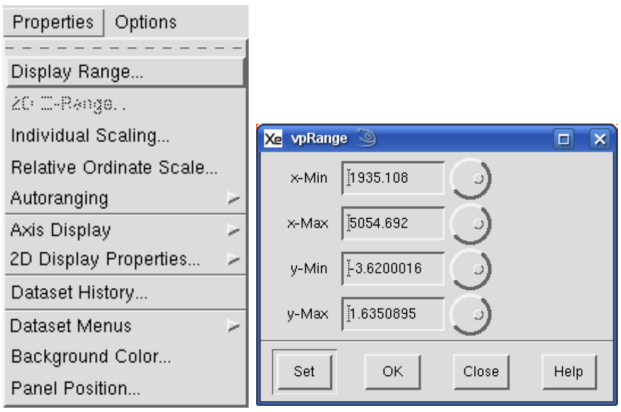


You can also use the X-Range*2, Y-Range*2, or X-Range/2, Y-Range/2 buttons in the Tool bar to zoom in or out by a factor of 2. The previous range button brings you back to the previous scale. The **FS** button brings the spectrum back to full scale in case you zoom in too much and get lost.



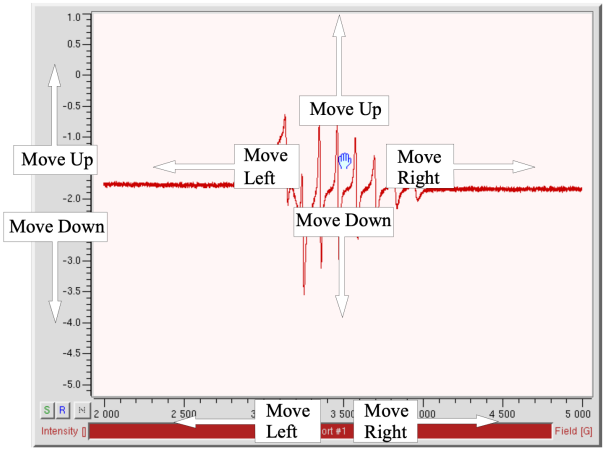
To display a precisely defined area you can click **Properties** from the menu bar and then **Display Range**.

A dialog box appears in which you can then select precisely the X- and the Y- range for display. Click the **Set button** in the dialog box to exe- cute the selected range.



Moving a Spectrum Around

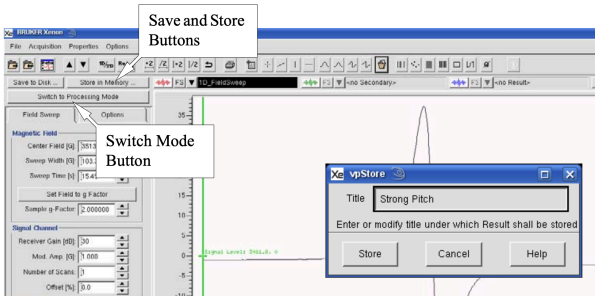
You can move the spectrum around by clicking the middle mouse button (scroll wheel) while the cursor is in the viewport display area and dragging the spectrum. The cursor changes to a move cursor. You can also place the cursor on either axis area to constrain the movement along one axis.



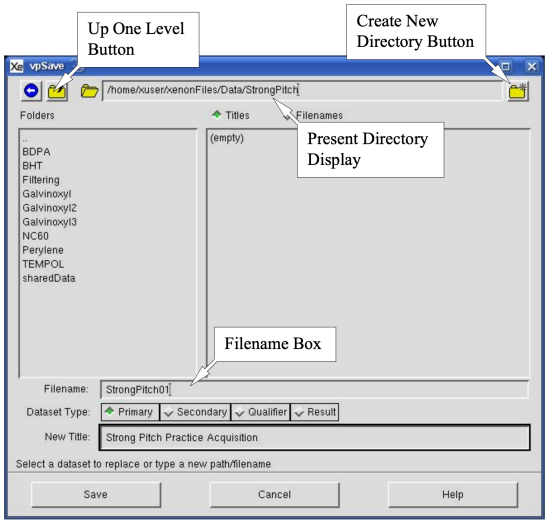
Storing and Saving the Spectrum

After you have acquired your spectrum, you may wish to save or store it. What is the difference between these two operations? The Store in Memory operation stores the spectrum *temporarily* in memory which means it is lost when you exit Xenon. The Save to Disk operation saves a *permanent* data file on the hard disk for future reference. Typically, Store in Memory is used to store intermediate results and Save to Disk is used to permanently save the results of your data acquisition or processing.

1. **Store your spectrum.** Click the Store in Memory button. The Store dialog box allows you to enter a descriptive title for the dataset. The presently active spectrum is stored in memory when you click Store. You may also notice that Xenon switches to Processing Mode. To return to Acquisition Mode, click the Switch Mode button.



2. **Save your spectrum.** Click the Save to Disk button. Enter a descriptive title for the dataset in the Title box. The Save dialog box lets you enter a filename and destination directory. All date should be saved in the **/home/xuser/xenonFiles/data** directory. Data saved anywhere else will be deleted and not archived. Enter the file name in the Filename box. **The file name must be of the format defined below or it will be deleted and not archived.** Clicking OK saves the presently active spectrum on the hard disk. Note that the spectrum is also stored in memory when saved.



File Name Format: *PI_YYMMDD-optional_description*. Example **pjp_220621-example**

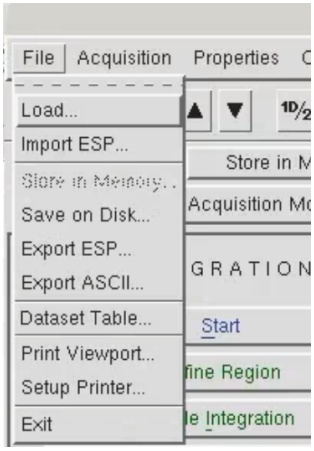
PI INITIALS ONLY! We use this for sorting archived datasets. The date code helps give a chronologic order and makes locating datasets easier. **All other file names will be deleted**.

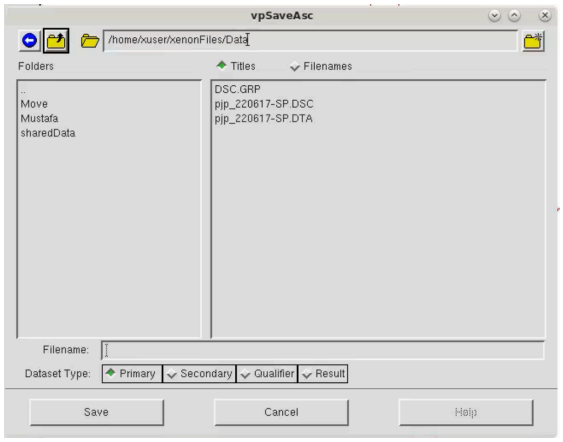
Generating Output for Figures and Reports

There are not many options for processing EPR results away from the instrument's workstation. Xenon is not available for download and other options either require Mathlab or do not have a graphic interface. However, there are three options for transferring datasets for use in publications and figures.

1. Exporting ASCII Text Files

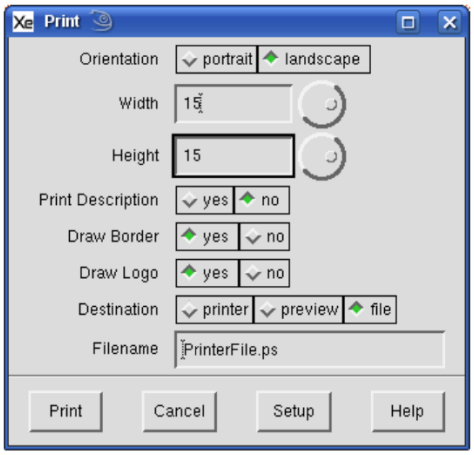
If you want to display the data using graphing software like Origin, you need to export the spectra in ASCII format. Click **File** in the menu bar and then **Export ASCII**. A dialog box will appear where you can choose the file name, location to store and the source dataset. Click **Save** to export the file and exit the dialog box. For ASCII files, you should use the file extensions: .txt or .asc.





2. Printing to File

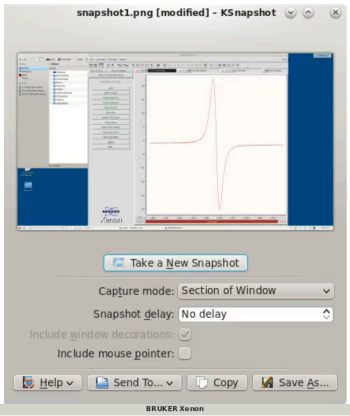
The system does not have a printer but you can generate plots to files that can be pasted into documents. Click the **Print button** in the toolbar near the top of Xenon. A dialog box then appears in which you can select the desired options. Make sure the **Destination** is set to "*File*" and select the other options shown in the figure to the right. Clicking **Print** creates the file in the xuser's "Home folder" and closes the dialog box.



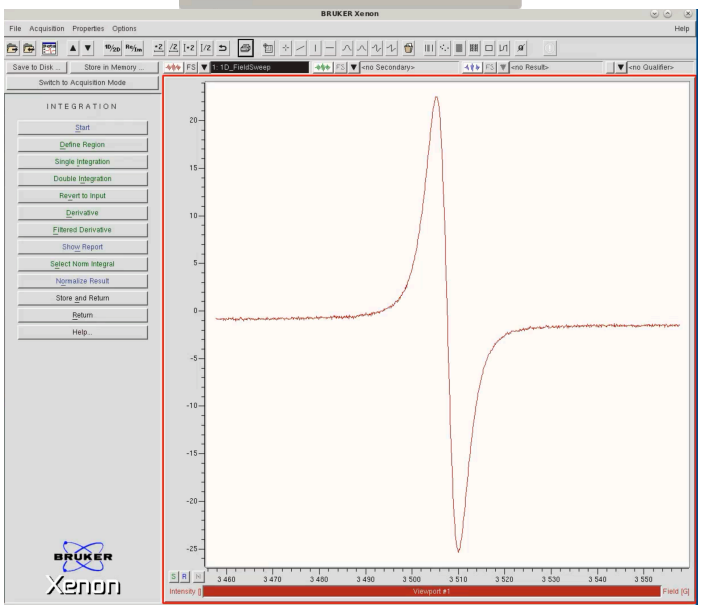
The file generated is a postscript file. Mac's will do a better job opening the files (Preview will convert them to a PDF file) than Windows computers. A graphics program like Inkscape or Illustrator might be necessary.

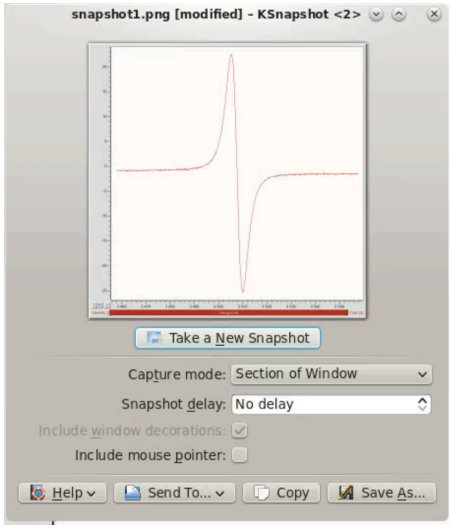
3. Linux Screen Snapshot

Pressing the keyboard's "Print Screen" button opens the Linux Screen Snapshot utility. Change **Capture mode** to "*Section of Window*" then click the **Take a New Snapshot** button. The dialog box will disappear.



Take the mouse cursor and point at the top left corner of the gray area of the Viewport that contains the vertical scale. A red box should surround the data window. Then double click with the cursor in this area and a new dialog box (below) will open.





Click on the "**Save As…**" button to save the image you generated. In the dialog box that opens you can choose a file name and select from a variety of image file formats. Then click the **Save** button.