# Endstation Operation and Data Collection Procedures

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# 1 Starting Endstation Software

## 1.1 Starting SPEC Software

1. Open a terminal and login to IOC by clicking "Run RIXS ES" on the desktop.
2. Start spec by typing *runSPEC*
3. SPLOT will start automatically; click the "Connect to SPEC" link.
4. Click "Remote"; ensure the dialogue box reads "spec" and "localhost", then click connect.

## 1.2 Starting Camera Software

1. Run the camera software by clicking the "RIXS_Cameras" icon.

# 2 Setup Mono

**Notes: You will only need to change mono mirrors and gratings if you require either more flux or resolving power for your requested energy. The EPU gap should be optimized by using *setEPU offset* and doing a *ct* to check the beam intensity. This is only necessary for when you have changed your energy range, not for a new sample.**

1. Use *moveM* to select the mirror and *moveG* to select the mirror for the desired energy range. Ensure that you select the mirror coating before selecting the grating.
   - There are charts on the wall to help with selection, if you unsure consult with beamline staff.
   - Generally, you can use the following:
     - Nickel mirror and Ni LEG when using 200 eV to 800 eV energy range.
     - Carbon mirror and Au LEG when using energy below 200 eV.
     - Silicon mirror and Au HEG pair when using energy above 800 eV.
   - For example,*moveM Carbon* and *moveG AuLEG*
2. Select the correct undulator harmonic and polarization using *setEPU harmo* and *setEPU polar*, respectively.
3. For example, *setEPU harmo 1* and *setEPU polar lh*
   - Generally, you can use the 1st harmonic, except when the energy is above 800 eV, use the 3rd harmonic.
   - The undulator polarization should be linear horizontal unless you are wanting scattering into the spectrometer for calibration or conducting XMLD and XMCD.
4. Use *moveE energy* to move the energy to your desired position.
   - For example, *moveE 500*
   - Consult the reference spectra figures to determine typical excitation energy. Alternatively, you can also consult the orange book. Usually, the excitation energy is set to 30-40 eV above above the absorption edge to start.
5. Ensure pressure in the endstation is less than $1.0 \times 10^{-8}$ Torr or less.
6. Open endstation valve and shutter
   - *setBEAM on*
7. Adjust undulator offset for maximum flux.

- First use *ct* to determine current count rates.
- The values for the TEY and I0 should be should be between 250,000 and 750,000 Hz
- The sensitivety of the SR570s can be set using *setAMP*. For example *setAMP a up* for SR50A.
  - a = Mesh Current (formerly I0)
  - b = Sample Current (formerly TEY)
- Set the EPU gap offset with *setEPU offset*
  - Typically this should 0.000 mm, but you can try an offset of $\pm$0.100 mm to see if more flux is realized.

8. Close endstation shutter
   - *setBEAM off*

# 3 Setup Spectrometer

1. Select grating based on energy range required, use *setXES grating*
   - For example, *setXES grating MEG*
   - Consult diagrams on wall for help with selection.
   - In the case of moving, if the grating does not report in place, try again. If the problem persists contact beamline staff.
2. *Use moveXES energy angle_defocus* to move the spectrometer to the desired energy
   - For example, *moveXES 500 0*
   - Consult beamline staff or diagrams on the wall if unsure about position
   - Ensure that after the move is complete the correct position is reported
   - Ensure that a correct shift file is loaded for the position, otherwise, contact beamline staff to generate a shift file. If you are planning to measure an edge without prior notification to beamline staff, you will have to shift the mcp image yourself in post-processing if beamline staff are unavailable.
3. Place the beam on sample using moving macros, *umvr ssh*, *umvr ssv* and *umvr ssd*
   - If you do not have a sample in the beamline that produces visible light, the default measure position is approximately the center of the sample plate in focus.
   - Turning off visible light sources will cause the cameras to switch to IR mode making the beam spot more easily visible.
     - ssh - sample horizontal; movement of the sample plate to the right is positive.
     - ssd - sample depth; movement of the sample plate to the rearward is positive.
     - ssh - sample vertical; movement of the sample plate upward is positive.
     - ssh - sample angle; movement increasing the angle of incidence is positive.
4. Ensure mask is in place using *setXES mask*
5. Using *ct seconds* take a test spectrum to check whether the emission line is centred in the spectrometer window, for example, *ct 10*
   - If you are not satisfied with the spectrum, adjust spectrometer centre and angle as necessary
   - Try to get the spectrum centred and have at least 5 eV on either side if possible.
   - If you increase the angle of the MCP too far you will start to clip the image.
6. Move the pin hole into place using *setXES pinhole*.
7. Using *setPIN*, centre the beam along the axis of the grating
   - Use *setPIN* to start, then add in an argument to shift the image, for example, *setPIN*, and then *setPIN 5*
   - Try to get the peak centred in the data plot.
8. Move the mask back into place using *setXES mask*

Now the beam is focused and aligned with both cameras. You can use in-plane moves to move between samples. Don't forget to add sample thickness with *umvr sdd* moves. If you are in doubt, you can check the alignment with the pinhole.

# 4 Collecting XAS Spectra

1. Use *newfile filename* to select your data file, please place multiple scans in each data file, for example, *newfile test.dat*
    - Use print DATAFILE to determine the current data file
2. Optimize SDD range and Mesh/Sample current amplifiers.
3. Ensure the excitation energy is 30-40 eV above the edge. Use *ct* to determine the count rates
4. Adjust the SDD count rate using the *setBL esgap*. For example, *setBL esgap 20* will set the exit slit to 20um.
    - Ideally, a good rule is to keep the count rate less than 30,000 cps when the energy is non-resonant. This will ensure the deadtime is less than 5%.
5. Once the SDD range is optimized, adjust the sensitively using *setAMP* of the Mesh/Sample current amplifiers (less than 1,000,000 Hz, again, above the edge 500,000 to 800,000 Hz should be okay).
6. Use *Escan start1 stop1 intervals1 stop2 intervals2 etc. dwell*
    - For example, *Escan 270 280 50 320 400 5* where the count time is 5 seconds, the spacing between 270 eV and 280 eV is 0.2 eV and 0.1 eV between 280 eV and 320 eV.

The total detector output will be plotted during the XAS scan. It is a good idea to watch the SDD MCA output for pileup during the scan.

# 5 Collecting XES Spectra

1. Use *newfile filename* to select your data file, please place multiple scans in each data file, for example, *newfile test.dat*. One can mix both XES and XAS scans in the same file.
    - Use *print DATAFILE* to determine the current data file
2. Ensure that you have not left the exit slit closed from previous XAS scans. Typically all XES measurements are completed using 25 um exit slit size.
3. Complete a *ct 30*
    - Ideally you would like to have a least 1000 peak counts. Calculate time accordingly.
4. Use *Tscan dwell total_time*
    - For example, *Tscan 30 300*, counts at 30s intervals for up to 5 minutes.

The XES spectra with be plotted in MCA form. Provided you have a valid shift file the plotted spectrum will be the final. If not, then there will be a loss in resolving power for the plotted spectrum. The user will have to process the image after the experiment. The XES spectrum is plotted in both, last exposure and total accumulated spectrum.
**Collect the correct data to generate your own shift file.**

1. Move the beam onto the copper sample plate, ensure the beams remains in focus. i.e. subtract sample height with a normal movement.
2. Change the beamline polarization to vertical down with *setEPU polar lvn*.
3. Move the beamline energy such that there is a scattering peak in the centre of the detector.
4. Collect XES spectra for each peak, pay attention to the requested excitation energy.
5. Repeat for scattering peak at either end of the spectrometer window.

If you pass this data on the beamline staff they can implement a shift file, but any data taken before this will have to be shifted in post-processing.

# 6 Plotting Data

The data plotting can be quite complex, and given the current stage of the user software, the visualization of the data is quite primitive. The following can be used to plot the data in Igor provided on the beamline computer.

- Create an appropriately named folder and make the folder active.
- Plotting .dat file
  1. Use ctrl+L to load a file. Ensure you deselect ”Load columns into matrix” and select ”auto name and go”.
  2. Click ”File..” and load in you desired file.
  3. Type ”Import_Scan(N)” - N is the number of scans in the file.
- Plotting .dat_sdd file
  1. Use ctrl+L to load a file. Ensure you select ”Load columns into matrix”.
  2. Click ”File..” and load in you desired file.
  3. Type ”Import_SDD(N)” - N is the number of scans in the file.
- Plotting .dat_mcpMCA file
  1. Use ctrl+L to load a file. Ensure you select ”Load columns into matrix”.
  2. Click ”File..” and load in you desired file.
  3. Type ”Import_MCP(N)” - N is the number of scans in the file.
- Plotting .dat_xeol file
  1. Use ctrl+L to load a file. Ensure you select ”Load columns into matrix”.
  2. Click ”File..” and load in you desired file.
  3. Type ”Import_XEOL(N)” - N is the number of scans in the file.
- Parse scan data.
  1. Type ”Parse_Scans(N)” - N is the number of scans in the file.
- Familiarize yourself with Igor or ask beamline staff for advice on specific plotting operations.

## 6.1 Saving SPEC plots

SPEC plots can be saved or ”detached” by holding down *cntl* and clicking the desired window. These will never close, so try not to accumulate too many.

**WHEN YOU LEAVE THE BEAMLINE FOR AN EXTEND PERIOD OF TIME, 2 HRS OR MORE, AND ARE NOT COLLECTING DATA. CLOSE THE ENDSTATION VALVE AND SHUTTER.**