

# McPherson/Princeton Raman Control Software

Developed for the Reznik Lab at the University of Colorado at Boulder  
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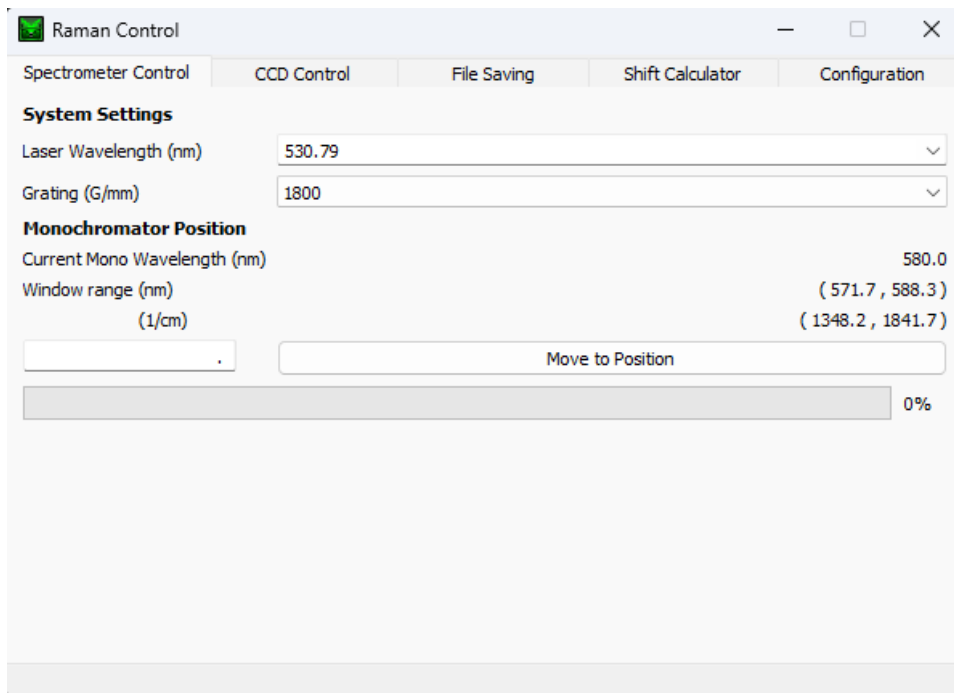


## Getting Started

- The PyLoN CCD must be cooled using liquid nitrogen before data can be collected. Carefully pour LN<sub>2</sub> into the dewar according to the PyLoN manual, being aware that some geysering may occur as the dewar walls cool down. It will take around 45 minutes for the detector to reach -120 °C. The detector should be on and the software should be running at the time so that the detector is not damaged by cooling below -120 °C.
- If the system has multiple users or has not been used in some time, it is recommended to perform monochromator (rough) and CCD (fine) calibration before taking data.
- Spectra at the current monochromator position can be obtained using the **1D spectrum** and **2D image** buttons, or live video from the detector viewed using the **Live Acquisition** section.
- The most recent spectrum/image can be saved to the desired folder and filename in the **File Saving** tab. All data is automatically saved in the Documents folder.
- The **Shift Calculator** tab provides a convenient calculator for Raman shifts.
- The **Configuration** tab contains calibration routines, settings, and useful troubleshooting information.

## First Tab: Monochromator Control

This tab handles control of the monochromator, which is used to select for different wavelengths/wavenumbers/energies.



The screenshot shows the 'Raman Control' software window with the 'Spectrometer Control' tab selected. The interface includes a 'System Settings' section with dropdown menus for 'Laser Wavelength (nm)' (530.79) and 'Grating (G/mm)' (1800). Below this is the 'Monochromator Position' section, which displays the 'Current Mono Wavelength (nm)' as 580.0 and the 'Window range (nm)' as ( 571.7 , 588.3 ). The wavenumber range is also shown as ( 1348.2 , 1841.7 ) in  $\text{cm}^{-1}$ . A text input field for a new position is followed by a 'Move to Position' button. At the bottom, a progress bar indicates the movement status, currently at 0%.

### System Settings

System settings include the current grating and laser in the system. These are preset to the last used values, but can be changed as desired.

NOTE: Recalibration of the CCD is required if these values are changed.

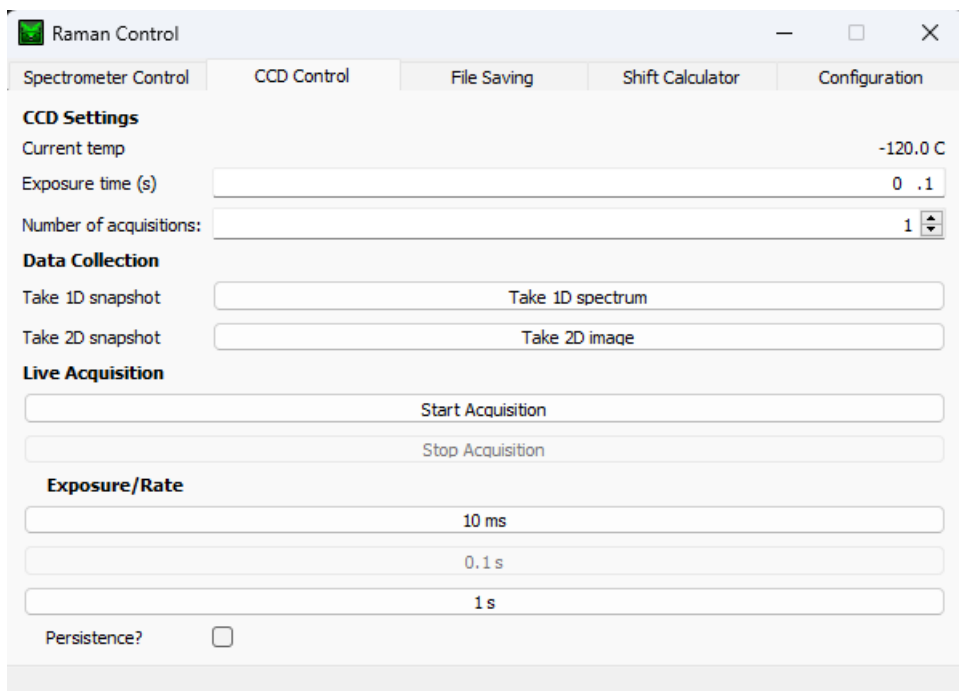
### Monochromator Position

The current monochromator position (center of the CCD window) is displayed in nm. For convenience, the rough bounds of the window in nm and  $\text{cm}^{-1}$  is displayed.

The monochromator can be moved by entering a new position (nm) and clicking *Move to Position*, with status of the movement monitored via the progress bar at the bottom.

## Second Tab: CCD Control

This tab handles control of the CCD imager which is used to collect data.



The screenshot shows the 'Raman Control' software window with the 'CCD Control' tab selected. The interface includes several sections: 'CCD Settings' with fields for 'Current temp' (-120.0 C), 'Exposure time (s)' (0.1), and 'Number of acquisitions' (1); 'Data Collection' with buttons for 'Take 1D snapshot' (labeled 'Take 1D spectrum') and 'Take 2D snapshot' (labeled 'Take 2D image'); 'Live Acquisition' with 'Start Acquisition' and 'Stop Acquisition' buttons; and 'Exposure/Rate' with three input fields (10 ms, 0.1 s, 1 s) and a 'Persistence?' checkbox.

### CCD Settings

CCD temperature is monitored and should be between -100 and -120 °C for best performance.

CCD exposure time can be changed. For bright samples, values 0.01—1s are sufficient; for dim samples, this can be set up to 9999 seconds (approx. 2.75 hours). This is longer than is supported by the PyLoN (2.3 hours) so care must be taken with particularly long scans to avoid unexpected behavior.

The number of acquisitions can be set between 1 and 199, with a default of 1. Multiple acquisitions will be taken sequentially and saved as one file.

## **Data Collection**

The software offers two measurement modes, which acquire a 1D spectrum or a 2D image from the detector. The former is intended to be the primary method of collecting high-quality data. The latter can be useful for alignment purposes. The spectral width of these images depends on the laser and grating used.

## **Live Acquisition**

Live data acquisition is useful for focusing and alignment. It can be started and stopped using the appropriate buttons. Upon starting, the selected framerate will be utilized; this can be changed without closing and restarting the live window.

Selecting 'Persistence' will take the median value for each pixel over a rolling 10-frame buffer, and can help reduce noise and the effect of cosmic rays.

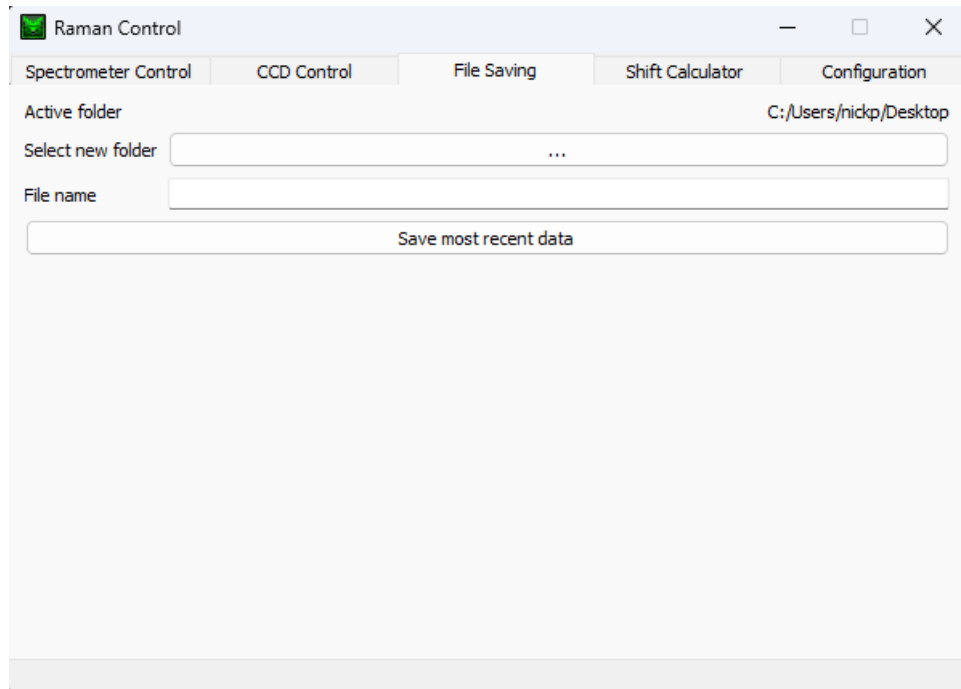
The view window can be changed by clicking and dragging on the live plot, or clicking on an axis and using the scroll wheel.

NOTE: Monochromator movement during live acquisition will cause unexpected behavior and should be avoided.

NOTE: The live window should be closed before taking data via the other modes, or else unexpected behavior may occur.

## Third Tab: File Saving

This tab handles file saving.

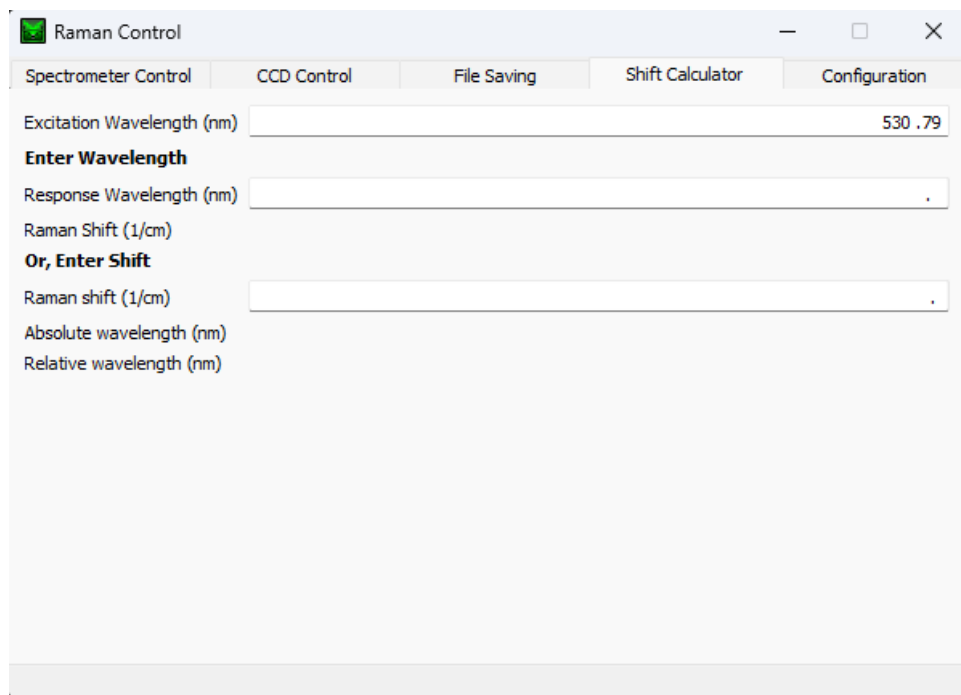


First, an active folder must be selected. This is the location that any selected data will save to. A valid file name (no extension) must be entered.

NOTE All data is saved to the Documents folder under a timestamp so that it may be recovered later if it is not saved manually.

## Fourth Tab: Shift Calculator

This tab provides a convenient means of calculating Raman shift, going from wavenumber to wavelength or vice versa.

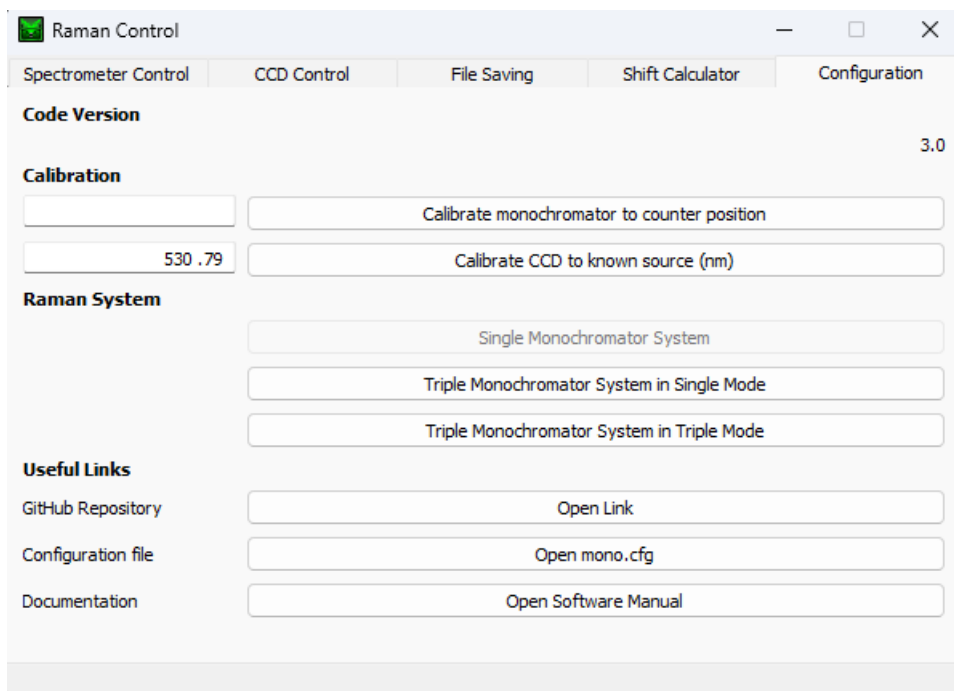


The screenshot shows the 'Raman Control' software window with the 'Shift Calculator' tab selected. The interface includes the following elements:

- Excitation Wavelength (nm):** A text input field containing the value '530 .79'.
- Enter Wavelength:** A section header.
- Response Wavelength (nm):** A text input field containing a decimal point '.'.
- Raman Shift (1/cm):** A text input field.
- Or, Enter Shift:** A section header.
- Raman shift (1/cm):** A text input field containing a decimal point '.'.
- Absolute wavelength (nm):** A text input field.
- Relative wavelength (nm):** A text input field.

## Fifth Tab: Configuration

This tab provides useful information and links.



The current code version is displayed and should correspond with the most recent available on GitHub and also with the current version of this manual.

### Calibration

Initial calibration of the software is performed by calibrating the monochromator position to the counter on the side of the device. This will provide a rough calibration in the event that the software position is off of actual position by more than about 1 nm. To do this, enter the current counter value in the blank box and click the calibration button next to it. This should not need to be done frequently, but is the first step in a full calibration routine if the x-axis of collected data is not behaving as expected, preceding the following CCD calibration.

NOTE: Counter and monochromator wavelength are related by a proportionality constant which is dependent on the grating, and accessible in the system manual.

Additional calibration of the CCD is necessary for the collection of high precision data. This relies on a known source such as a laser or gas discharge lamp, and centers the peak wavelength at the known (expected) position. If calibrating to the laser line, the laser must be on and aligned, and ideally attenuated by a strong ND filter but no spectral-shaping filters. This is done to avoid blowing out the detector. Calibration spectra are saved in the Documents folder.

NOTE: The CCD calibration routine must be performed if the grating or laser has been changed since this was last performed.

### **Raman System**

This section allows selection of the system in use. Currently, the triple monochromator system in triple mode is currently not supported. This may be added later down the line.

### **Useful Links**

This section contains links to the GitHub repository, where underlying code and files are hosted; the configuration file, for manual updating or verification of the values housed there; and this software manual.



## Appendix

### Technical Information

- This software is developed in Python, using the PyQt (Qt for Python) and pyblib libraries, and packaged into an \*.exe using auto-py-to-exe
- PICam drivers from Teledyne are essential for operation
- Communication with the PyLoN is over GigE
- Communication with the monochromator(s) is over serial (COM) and uses Serial to USB adapters requiring ftd2xx drivers in multiple locations within the C:/ drive

### Troubleshooting

- If the program fails to connect to the monochromator, ensure that in `mono.cfg`:
  - For the single monochromator system,  
`mono_system = single`  
`com_port = COM3`
  - For the triple monochromator system operating in single mode,  
`mono_system = triple_single`  
`com_port = COM1`
- In rare circumstances, `mono.cfg` may be left blank, which will prevent the software from operating. In such a case, a new copy of the file should be acquired from GitHub, and replace the blanked one. The software will have to be recalibrated and the correct values for all parameters re-established.