McPherson/Princeton Raman Control Software

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Getting Started

- The Princeton PyLoN CCD must be cooled using liquid nitrogen before data can be collected. To do so, carefully pour LN_2 into the dewar using a funnel according to the PyLoN manual. It will take around 45 minutes for the detector to reach -120 °C.
- It is recommended that the monochromator (rough) and CCD (fine) calibration be performed when the program is first started, especially if the system has multiple users or has not been used in some time. This should only need to be performed once, however CCD calibration may be useful to do more often to ensure high-precision data is being collected.
- Spectra at the current monochromator position can be obtained using the **1D spectrum** and **2D image** buttons. Wider spectra can be obtained by entering start and stop wavenumbers and using the **Raman spectrum** button.
- Live spectra at the current position can be taken in the **Live Acquisition** tab, with a few framerates available.
- 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.

First Tab: Monochromator Control

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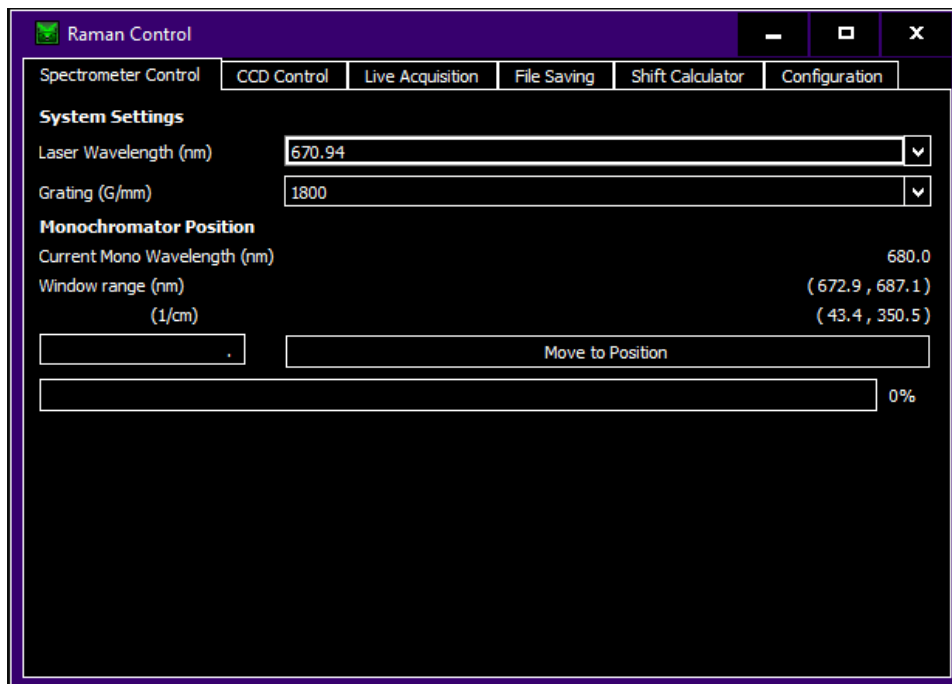
System Settings

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.

Monochromator Position

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

NOTE: If laser or grating is updated, these values will not be accurate until CCD calibration is performed. For more information on this, see the **Configuration** section.

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 PyLoN CCD is cooled by liquid nitrogen. Carefully pour LN_2 into the dewar according to the PyLoN manual, being aware that some geysering may occur as the dewar walls cool down. Also, LN_2 can easily spill out of the funnel if it is filled too quickly. Slow pours or small amounts at a time are recommended. Cooling of the CCD from room temperature takes about 45 minutes.
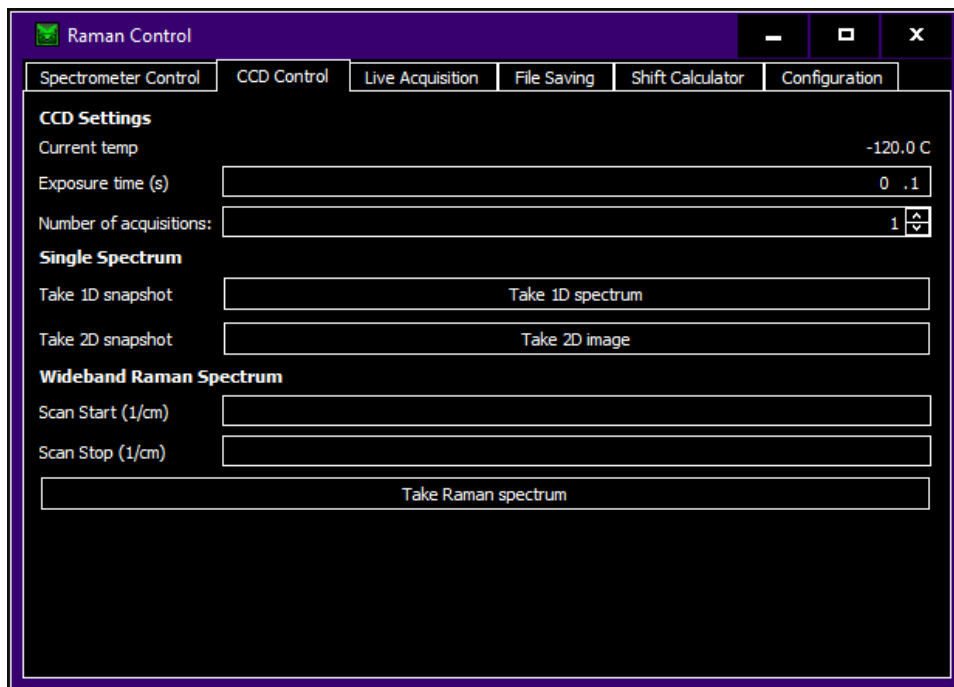
CCD Settings

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.

Single Spectrum

The software offers two snapshot 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.

Wideband Raman Spectrum

There is also an imaging mode for wider spectra, primarily intended for general mapping of the Raman spectrum for a sample. This works by taking spectra at different monochromator positions and then stitching them together. There may be some gaps/overlaps in the resulting spectrum, and peak amplitudes may be slightly misrepresented.

Third Tab: Live Acquisition

This tab handles control of live data acquisition for focusing and alignment purposes.

Live data acquisition (video mode) 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. Limits for the x-axis (cm^{-1}) and y-axis (counts) can also be set to allow for easy inspection of a particular region of interest. Clearing these limits will not reset the view, which may only be possible by closing and reopening the live window.

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

NOTE: The live window should be closed before otherwise taking data, else unexpected behavior may occur.

Fourth Tab: File Saving
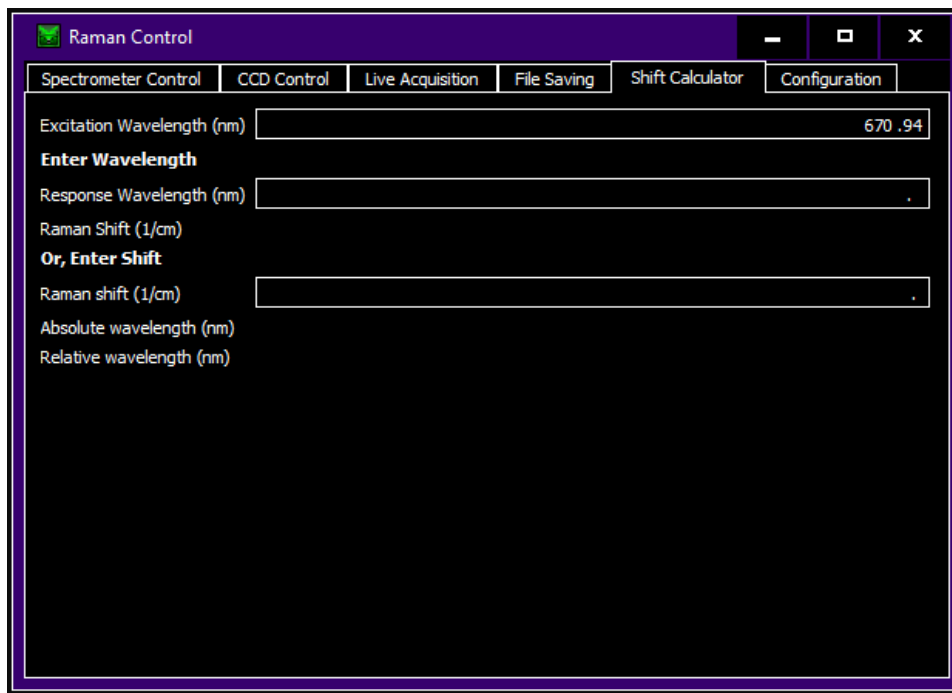
This tab handles file saving.
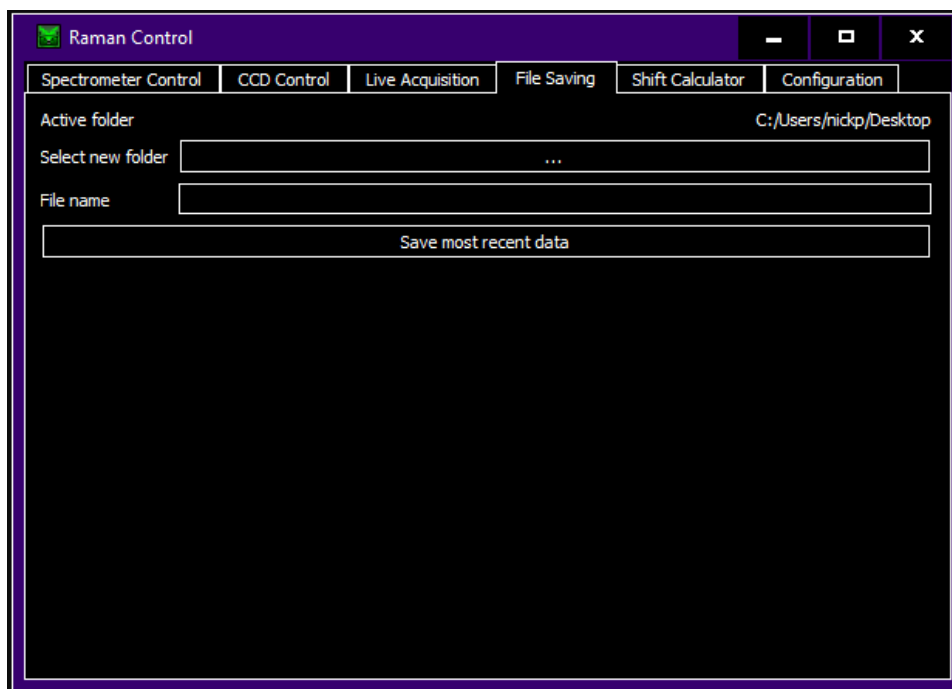
First, an active folder must be selected. This is the location that any selected data will save to. A valid file name (no extension) must be entered.

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.

Fifth Tab: Shift Calculator

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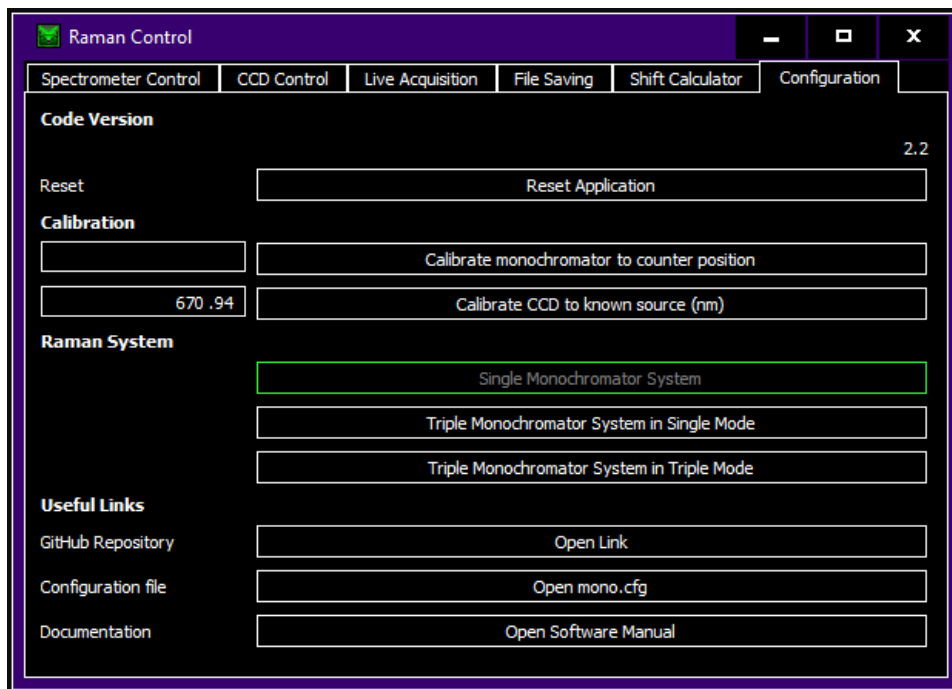
Sixth Tab: Configuration

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.

A reset button is provided which will reinitialize the application in the event of an error, notably the "Acquisition not in progress" error that may come with multiple acquisitions.

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.

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 pylablib libraries, and packaged into an *.exe using auto-py-to-exe
- PICam drivers from Teledyne are essential for operation
- Tracking of the *.exe in GitHub is done using git lfs
- 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`

- The "Acquisition not in progress" error occurs occasionally. This may cause strange behavior, but should be resolved using the *Reset* button in the **Configuration** tab. This error may be most common when a large number of acquisitions are requested, especially for short (<1s) exposure times. An error during a serial acquisition will lead to a smaller number of frames being obtained than expected.
- 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.