SFG Spitfire Workup Guide

**Introduction:**

This workup is heavily based on Paul’s SFG Solstice workup with a few adjustments tailored to the Spitfire setup. It does include some minor additions (final\_correction.py) that allows one to complete all the workup in Python including normalizing to gold spectrum and calibrating to polystyrene wavenumbers. Background scan of the sample spectrum now saves by default since Franz asks about it so often.

The Python IDE Spyder is recommended here because it’s pretty.

Here is the link: (<https://www.anaconda.com/download/)>

**Preparation:**

In the script package you will find a folder for inputting data (data\_input) and one for outputting data (data\_output):

* Make sure your raw experimental data files are copied into data\_input before proceeding to the workup.
* Make sure files for each run of an experiment are in their separate folder, so that the script doesn’t sum the same DFG position from different runs of an experiment.
  + e.g. files for SFG spot 1 of my sample are in: /data\_input/07082020/expt/run1
* In the execution folder (exe), there should be 5 scripts in total and the following are their functions:
  + **fullwn.py** : holds all the wavenumber values that the acquisitions, once they are padded with zeros and/or properly summed up, are plotted against.
  + **acq\_dfg.py** : ﻿holds data from a single or multiple frames of DFG acquisition
  + **spectrum.****py** : holds methods to subtract, filter, pad, truncate, sum, plot, and then write to get to the final spectrum
  + **import\_data\_here.py** : plots the truncated and summed gold (if not already) and sample spectrum and writes the datapoints into a txt file
  + **final\_correction.py** : normalizes sample signal to gold signal, and calibrates wavenumber to the polystyrene 2850 and 3060 cm-1 peaks. This script does what we manually do before in Igor after acquiring the summed gold/sample file

**Workup** **Procedure:**

Module loading sequence:

* + fullwn.py
    - if CCD camera is shifted during your experiment, make sure you change the “standard” file to a gold file taken during your experiment
  + acq\_dfg.py
  + spectrum.py
  + import\_data\_here.py
    - make sure the input path is set to where your experimental files are located, and output path is set as desired
      * e.g.

﻿input\_path = '/Users/ricoxi/Desktop/Spitfire/data\_input/'

output\_path = '/Users/ricoxi/Desktop/Spitfire/data\_output/'

* + - under the input/output path, set **gold** and **sample** to the folders where the corresponding files for gold and sample are
      * e.g.

gold = '20180124/endAu'

sample = '20180124/expt/lipidspec'

* + - name your file as desired, you do not need to include filename extension
      * e.g.

gold\_name = 'test\_gold'

sample\_name = 'test\_sample'

* + - once run, check the plots in the “plot” window. If everything looks right, proceed to the next part
  + final\_correction.py
    - make sure **output\_path** is set as desired
      * e.g.

output\_path = '/Users/ricoxi/Desktop/Spitfire/data\_output'

* + - make sure the **sample\_name** from the “import\_data\_here.py” is the same, and re-defined somewhere in the script
      * e.g.

sample\_name = 'test\_sample'

* + - name your final normalized and calibrated file to **cal\_name**
    - once run, check the plots in the “plot” window. If the spectrum is correctly shifted, you are done!
      * **IF NOT**: go to the “**PS** **local minima**” plot and find the correct index for dots representing the 2850 and 3060 dips. Manually change **loc1** and **loc2** to the correct index according to the plot. There should also be a prompt in the “console” window telling you where the script thinks the minima are at, check to see if it fits your expectation.

**Help:**

* ﻿"DFG stands for 'difference frequency generation'. When collecting a broad SFG

vibrational spectrum, the IR wavelength and detector wavelength need to be

shifted across frequency space as they are too narrow to do everything at one time. The IR wavelength is shifted by changing the position of something called

the DFG crystal, hence the name of a single one of these acquisitions."

--pohno

* There are many functions in the **spectrum.py** file you can call if you need to do specific things
* Tbd…