OCD Analysis Software (v 1.0)

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This software is designed to plot and process spectra obtained from the J-810 Jasco CD spectrometer in the Huang lab. All measurement files must be in ASCII format (*.txt files). This format can be chosen when saving the measured spectra in the Spectra Manager software provided by Jasco. File reading routines are currently optimized for J-810 ASCII output, though these can be modifed to read any consistent text-based spectral data file.

The software is designed to work as a collection of tools, so that it may be used interactively. To start an interactive python session, type the folloing command at your shell or command prompt:

```
>_ python
Python 2.7.13 (default, Dec 17 2016, 23:03:43)
[GCC 4.2.1 Compatible Apple LLVM 8.0.0 (clang-800.0.42.1)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>_
```

Depending on your distribution and machine details, the output above may not be exactly the same (This output was generated on a 2015 Apple MPB with a brew install of python 2.7). Next, the tools must be imported:

```
>>> from ocd import *
```

This also imports the following python modules: numpy as np, and matplotlib.pyplot as plt. Loading a spectrum is done through the creation of a instance of the class ocd_spec. Providing a filename loads the corresponding spectral information (wavelength and CD signal). Optionally the class may be called without a filename to create an empty spectrum (no spectral information):

```
>>> myspec = ocd_spec("scan_01.txt")  #class with filename
>>> emptyspec = ocd_spec()            #empty class
```

Once a spectrum is loaded, you have access to the following functions and variables:

ocd_spec.wl : returns a 1D numpy array of wavelengths used in the scan

ocd_spec.cd : returns a 1D numpy array of CD signals measured

ocd_spec.load(string) : loads wl and cd data from specified filename

ocd_spec.name(string) : changes the name of the spectrum

ocd_spec.graph() : produces a simple graph of the spectrum

ocd_spec.renorm(float) : globally rescales the CD signal by specified factor

avg_signal([spec1, spec2, ...]) : returns an ocd_spec class with an average CD signal from spec1,spec2, ... The spectra must be passed to this function as a python list.

In this way, multiple spectra can be graphed, rescaled, and analyzed interactively at the user's discretion. Custom graphs (custom color schemes, plotstyles, line types, etc.) can be made by directly calling functions from the pyplot module:

```
>>> fig = plt.figure("Custom Plot")
>>> plt.plot(myspec.wl, myspec.cd, 'b--',linewidth=2)
>>> plt.xlim(220,240)
>>> plt.title("230 nm Peak - A State")
>>> plt.ylabel("CD [mdeg]")
>>> plt.xlabel("Wavelength [nm]")
>>> plt.show()
```