VISION Data Reduction Guidelines

How to access VISION data:

- Log on to the analysis cluster at http://analysis.sns.gov and click *Launch Session*. Enter the username and password for your ORNL Resource Account (created at the ORNL Guest Portal).
  - Alternatively, there is a dedicated data analysis computer in the VISION hutch that can be used to access the analysis cluster.
- Open the *Caja* file browser by clicking on the icon or on your home folder (see picture below). Data measured during the experiment is located in data/SNS/VIS/IPTS-XXXXX/shared/manualreduce, where XXXXX is the IPTS experiment number.
  - It can also be found in /SNS/VIS/IPTS-XXXXX/shared/manualreduce.
  - Data are listed by the run numbers
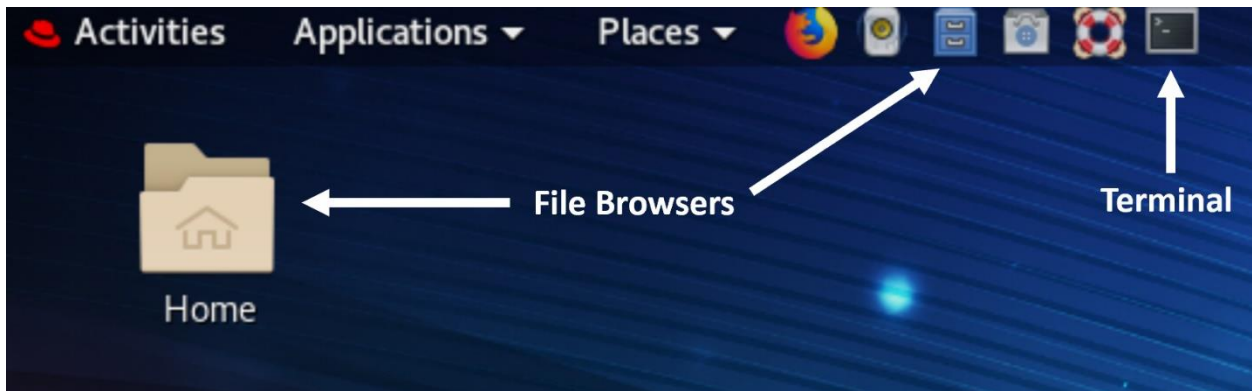
Using *Mantid Workbench*:

- Open up *Mantid Workbench* by clicking the *Applications* tab → *Analysis* → *Mantid Workbench*. This can also be done by entering the *mantidworkbench* command in the terminal window
- A window will pop up. Set the default instrument to VISION.
- Optional: Choose the default directory to save your data. Click the *Manage User Directories* button. In the *Default Save Directory,* enter the path that you want your reduced data to be saved. Press *OK.*
  - This window can be found later using *File* → *Manage User Directories*
- The main *Mantid Workbench* window is displayed below.
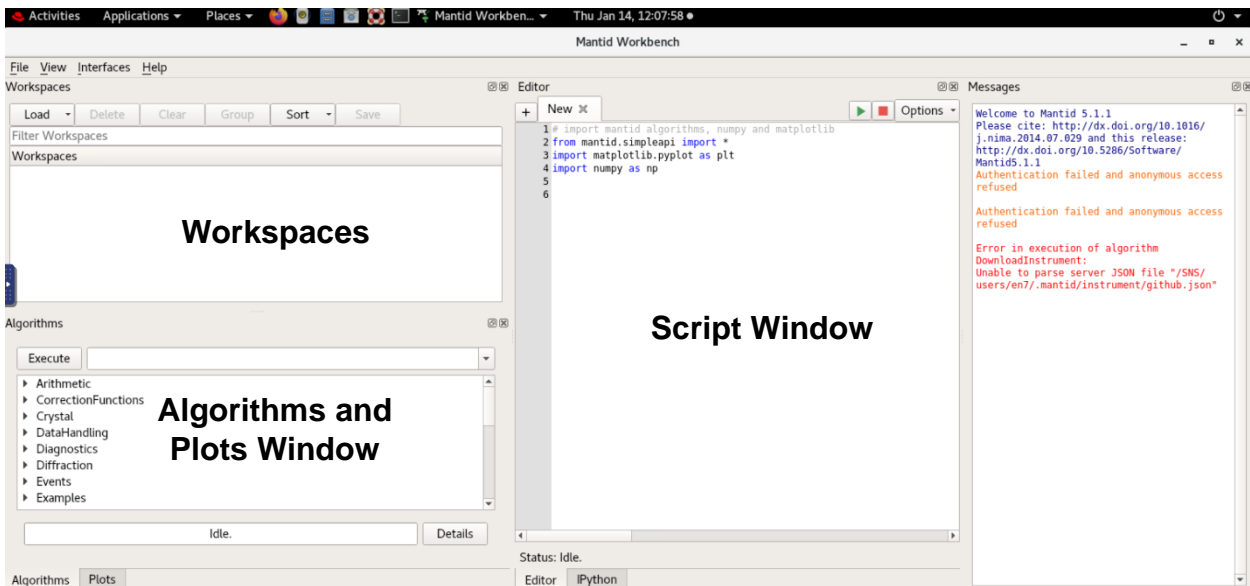
- o The *Algorithms* window contains a list of algorithms that can be used to modify the data manually (scaling, unit conversions, loading files, saving data in different file formats, etc.).
  - For detailed information about the algorithms, click on *Help → Algorithm Descriptions*.
- o The *Plots* window will display plots generated from the data.
- o Toggling between the *Algorithms* window and the *Plots* window can be achieved using the *Plots* and *Algorithms* tabs located below the Algorithm and Plots Window.
- o The *Workspaces* window contains the data files.
- o The *Script Window* displays the python scripts used to reduce VISION data.

Inelastic Data Reduction:

- Python scripts are used to reduce the data at VISION.
  - o The local and global parameters that are executed in the script are the same as the corresponding algorithms found in the *Algorithm* search bar.
- To open a script, click on *File →* Open Script and navigate to /SNS/VIS/shared/VIS_users/scripts/. This contains a list of scripts used to reduce VISION data. Open vis_analysis.py.
  - o Save a new copy of vis_analysis.py in a different directory.
    - We recommend saving this script in your experiment folder (data/SNS/VIS/IPTS-XXXXX/shared/manualreduce directory).
- An example of the python script is shown below. Users should only need to modify the file below line 8. The following will explain the main sections that may need to be modified during the data reduction process.

```
vis_analysis_tutorial_2022.py*   ×                                                          ▶ ■ Options ▼

 1 from mantid.simpleapi import *
 2 import sys
 3 sys.path.insert(1,'/SNS/VIS/shared/VIS_users')
 4 import vis_module
 5 from vis_module import *
 6 d= []
 7
 8 #========control block========
 9 file_structure = 'IPTS'  # IPTS: IPTS subfolders. Flat: flat structure, all data under the root dir
10 root_dir = '/SNS/VIS'
11 raw_subdir = 'nexus'     # needed only for file_structure='IPTS' and pc_weight=True
12 reduced_subdir = 'shared/manualreduce'  # needed only for file_structure='IPTS'
13 pc_weight = False        # True: spectra weighted by proton charge, raw data needed for proton charge. False: need reduced data only, good for most cases but
14 save_flag = 0            # 0: No output saved.  1: processed spectra saved in nxs and ascii
15 #========global parameters=====
16 scalex = 1.0; scaley = 1.              # scaling parameters for x (energy transfer) and y (intensity)
17 shiftx = 0.0; shifty =  0.             # shift along x and y (after scaling)
18 bin = '-2,0.01,5,-0.002,200,-0.005,1000'      # binning parameters
19 smooth = 0                             # smooth parameter NPoints (0 for no smoothing)
20 unit = 'meV'                           # 'cm-1' for wavenumber
21 #========data block==========                       # all the above global parameters can be overwritten in the data block (redefined for a particular dataset)
22 #d.append( DataSet('16502-', 'b', temperature, bin='', smooth=, unit=, scalex=, scaley=, shiftx=, shifty=) )
23
24
25 d.append( DataSet('56140-', 'b', scaley=1.2) )   #empty can
26 d.append( DataSet('55466-', 's', 5) )     #LaB6
27
28 #========================
29 [all_merged,all_bose,all_subtracted,all_bose_subtracted]=process_all(d,file_structure,root_dir,raw_subdir,reduced_subdir,pc_weight,bin,smooth,scalex,scaley,shi
30
```

- o Line 13: Controls which type of files is read and reduced. For most situations, we will be using pc_weight = False to use the auto-reduced files.
- o Line 14: Controls whether the files generated are saved or not when the script is executed.
  - ▪ Save flag = 0 will not automatically save the processed data. These files will be loaded into the *Workspaces* in the Mantidplot window and can be saved later in the desired formats using the *Algorithms* tab.
  - ▪ Save flag = 1 will automatically save the processed data in .nxs and ascii format to the working directory.
- o Lines 16-20 define the global parameters. These parameters will be used unless a local parameter is defined specifically in the data block (further explained below).
  - ▪ Lines 16 and 17 control scaling and shifting of the data.
  - ▪ Line 18: Controls how the data is binned. This allows for finer or coarser energy binning across different energy transfer ranges.
    - • The example shows a coarse bin size (0.015) between -2 – 5 meV, a fine bin size (0.003) between 5 – 200 meV, and coarser again (0.005) for 200 – 1000 meV.
  - ▪ Line 19: Smooths the data. Use 0 for no smoothing and 3 or greater for smoothing.
  - ▪ Line 20: Outputs data in either meV or wavenumber (cm^{-1}).
- o The data block (Lines 25 and 26) is where the specific data sets are loaded and modified.
  - ▪ Enter the run number for the data set that you want to reduce.
    - • To load a single file, just enter the run number ('40782').
    - • To combine a series of files, enter the run numbers separated by a comma ('40782,40789,40792')

- Long measurements are often split up into shorter runs, such as a two hour measurement that is split up into 4 different runs (30 minutes each). These runs will be given the same name, such as CaF_2_6mm_PAC_can_10x20_slits_5K, but the run numbers will be different. To load and combine all these files, simply include a dash after the run number of the first file in the series ('40782-') and the script will find and combine these files with the same name.

- Designate whether the data is a sample or a background measurement.
  - 's' marks the data as a sample measurement.
  - 'b' marks the data as a background measurement, which is typically an empty can. The background will be subtracted from the sample measurement.
  - Note: once a background measurement is defined, any sample listed subsequently will be background subtracted using that dataset unless a new background is defined.
    - In the example below, line 26 will use line 25 for a background. A new background is defined in line 28 and is now used for lines 29 and 30.

```
25 d.append( DataSet('56140-', 'b', scaley=0.90) )    #empty can
26 d.append( DataSet('55466-', 's', 5) )     #LaB6
27
28 d.append( DataSet('56150-', 'b', scaley=0.95) )    #empty can
29 d.append( DataSet('56155-', 's', 5) )     #Carbon
30 d.append( DataSet('56157-', 's', 100) )    #Carbon
```

- To correct the spectra for temperature, a Bose-Einstein factor can be applied. This is useful to compare datasets collected at different temperatures. To apply the correction, define the sample temperature by entering the number in kelvin units. The example (line 26) shows that the sample was measured at $T = 5$ K.
- Local parameters can be defined for each measurement, which will override the global parameters. A list of how to define each local parameter is shown in Line 22.
 - Line 29: Performs the VISION data reduction algorithm.

Example of VISION Inelastic Data Reduction:

- The script on Page 3 will reduce the data for a LaB_6 sample measured in a 6 mm diameter vanadium PAC can at 5 K.
- To execute the script, click on the *Green Play Button* or press Crtl + Shift + Enter.
- The *Workspaces* window is now populated with 5 different data sets.

Workspaces
▶ BOSE_NBG_VIS_55466-55468_alignment_LaB6_6mm_V_can_slits_10x50_at_5K-VIS_56140-56141
▶ BOSE_VIS_55466-55468_alignment_LaB6_6mm_V_can_slits_10x50_at_5K
▶ NBG_VIS_55466-55468_alignment_LaB6_6mm_V_can_slits_10x50_at_5K-VIS_56140-56141
▶ VIS_55466-55468_alignment_LaB6_6mm_V_can_slits_10x50_at_5K
▶ VIS_56140-56141_empty_6mm_V_can_slits_8x50_at_5K

- o VIS_run#... is the background and sample data sets.
- o NBG_VIS_run#... is the sample measurement with the background subtracted. NBG stands for no background.
- o BOSE_VIS_run#... is the sample with a Bose temperature correction.
- o BOSE_NBG_VIS_run#... is the sample with both a Bose temperature correction and the background subtracted.
- To plot the spectrum, right click on the desired workbook and click *Plot →Spectrum*.
  - o A window pops up and asks which spectra numbers to plot. VISION data is divided into three data sets, numbered 0, 1, and 2. These numbers are at the end of the file name when plotted, as observed in the Legend in the spectra below.
    - ▪ sp-0: High Q data (backscattering detector banks)
    - ▪ sp-1: Low Q data (forward scattering detector banks)
    - ▪ sp-2: Average of both low and high Q data
- The inelastic signal is very weak compared to the high intensity elastic peak centered at ΔE = 0 meV. Once the plot is generated, you will have to zoom in to observe the inelastic signal. The axes can be scaled by double clicking on the axis and changing the values in the dialog box. Likewise, you can click the magnifying
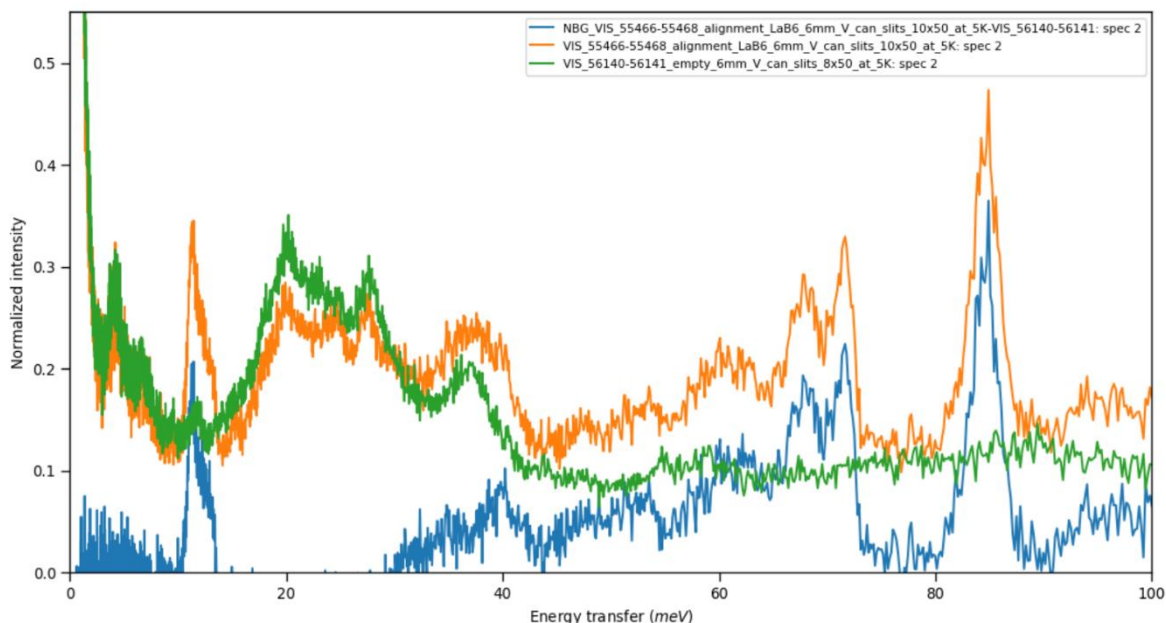
glass button to manually zoom into an area of the graph by drawing a box on the graph. A third way is to click the *Options Menu* button on the plot window.

- For this example, we will just use the average of high and low Q data (sp-2) without Bose correction.
- Plot the sample, background, and NBG sample on the same graph.
  - Once a graph is plotted, other data sets can be added by dragging and dropping a workspace onto the graph window.
- Zooming in on the low energy transfer region (<100 meV), we can observe that (1) the data is rather noisy and (2) the background is over-subtracted.
  - First, we will increase the bin size and smooth the data to reduce the noise. Change lines 18 and 19 to the following values:

    ```
    18 bin = '-2,0.035,5,-0.005,200,-0.005,1000'
    19 smooth = 3
    ```

  - Binning and smoothing parameters are determined on a case-by-case basis. This depends on the statistics, how sharp or broad the features are in your data, what information you are looking for, etc. Try adjusting both of these parameters to determine what works best for your data.
    - If the bin size is too coarse or too heavily smoothed, the data will look good but subtle features will be washed out of the data. If you are interested in broad features, you can get away with this type of treatment.
    - You can also plot the error bars to better determine if features are real or an artifact of noise.
  - As observed, the data is now significantly cleaner. Next, we need to scale down the background to correct for the over-subtraction.
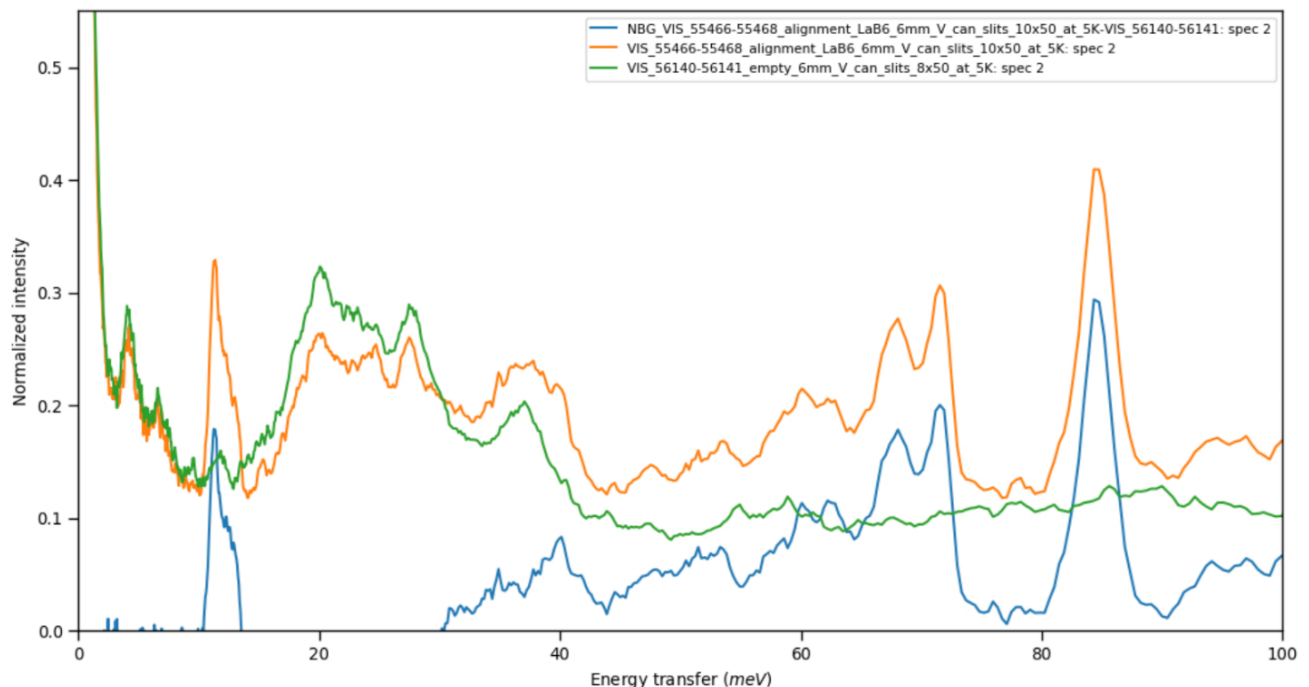
- The vanadium PAC cans produce a very small signal compared to most sample signals. Other sample cans (aluminum, steel, etc.) will produce more significant signals and need to be more carefully subtracted. Most of the signal from the vanadium can (green curve) consists of broad bands located below 40 meV. This is the region that you should focus on when subtracting the empty vanadium cell.
  - To correct the over-subtraction, change the local parameter *scaley* for the background data set to scale it to 0.9.

```
25 d.append( DataSet('56140-', 'b', scaley=0.90) )    #empty can
26 d.append( DataSet('55466-', 's', 5) )       #LaB6
```

- The background subtraction now looks reasonable in terms of intensity. The vibrational modes of the empty can also agree well with the features in the sample measurement, so the background measurement does not need to be shifted in energy transfer (*shiftx*).
- Data scaling, background subtraction, and many other data manipulation procedures can also be performed in the *Algorithms* tab in *Mantid*, rather than using the python script. For example, these commands can be executed by typing *Scale* or *Minus* in the *Algorithms* search bar.
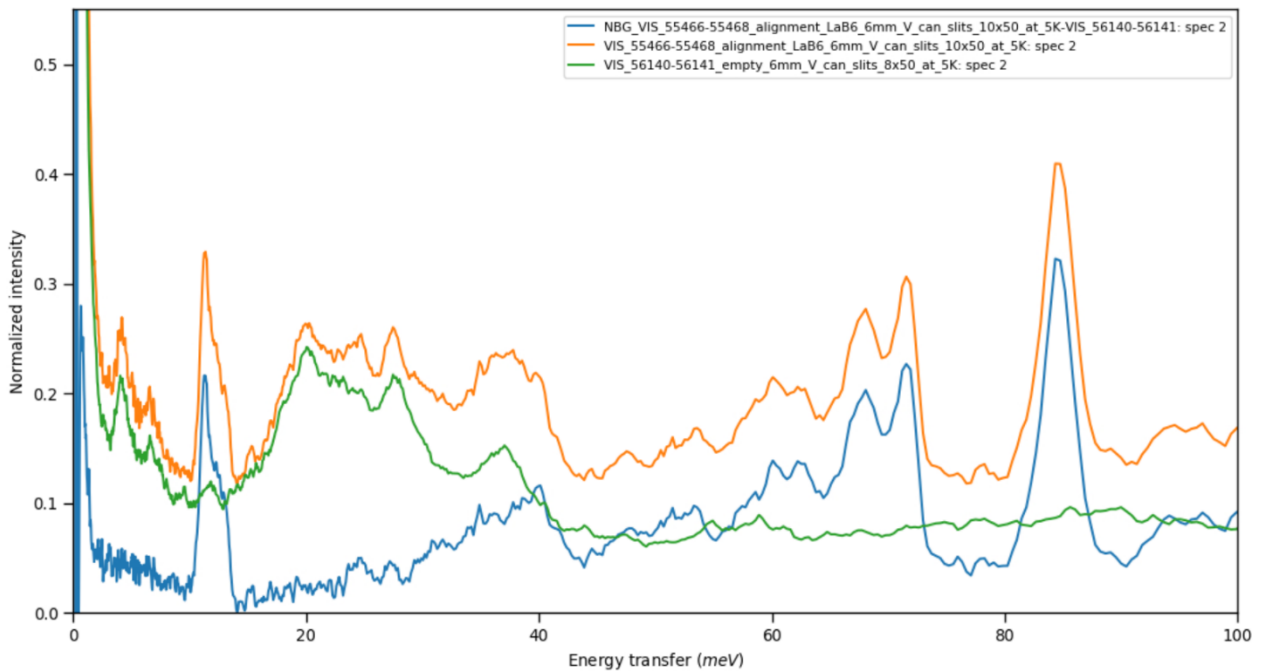
Saving Mantid Projects and Ascii Data Files:

- To save the *Mantid* project, go to *File → Save Project As* and define the path where you want to save it. Click *OK* to save.
  - This will save a mantid project file (.mantid) along with nexus (.nxs) files for each of the data sets in the *Workspaces* tab.

- To save data in ascii format, click on the *Algorithms* tab and enter *SaveAscii* in the search bar. Pick the workspace that you want to save. Define the path and filename for the save location. Pick which form of separator you would like to use (space, comma, etc.) Click *Run*.

- A .dat file has now been saved in the directory. It is in XYE format (energy transfer, intensity, error).
    - The three data sets (sp-0, sp-1, sp-2) are listed consecutively in the file. They are separated by the number of the data set beginning with 0, as seen below.

```
# X      Y      E
0
-1.9825 0.0623417 0.00892324
-1.9475 0.0728037 0.00976966
-1.9125 0.0669234 0.00931123
-1.8775 0.0781225 0.00993749
-1.8425 0.0734921 0.00966955
-1.8075 0.0905023 0.010683
-1.7725 0.0738415 0.00962638
```

Diffraction (Elastic) Data Reduction:

- The python script used for reducing diffraction data at VISION is located at /data/SNS/VIS/shared/VIS_users/scripts/vis_eed_analysis.py.
    - Again, we recommend saving a copy of this file to your experiment folder.

- The overall structure of the script is very similar to the inelastic data reduction script shown previously, but the calculation is different.
- Line 23: Controls whether the unit for the data is reduced in terms of d-spacing, momentum transfer (Q), time of flight (TOF), or wavelength.
  o This can also be done manually using the *ConvertUnits* algorithm and by setting *Emode* to *Elastic* in the *ConvertUnits* Window.

```
vis_analysis.py*  ✕    vis_eed_analysis.py*  ✕                                           ▶ ■  Options ▾

 1 from mantid.simpleapi import *
 2 import sys
 3 sys.path.insert(1,'/SNS/VIS/shared/VIS_users')  # path to vis_eed_module.py
 4 import vis_eed_module
 5 from vis_eed_module import *
 6 dict={};d=[]
 7
 8 #=========control block================
 9 file_structure = 'IPTS'  # IPTS: IPTS subfolders. Flat: flat structure, all data under the root dir
10 weight = 0               # 0: from raw file. 1: from reduced file. 2: from log file. 3: from error
11 save_flag = 0            # 0: output not saved.  1: processed spectra saved in nxs and gsas
12 root_dir = '/SNS/VIS' # root directory to the data files
13 raw_subdir = 'nexus'    # needed only for file_structure='IPTS' and weight=0
14 red_subdir = 'shared/diffraction'  # needed only for file_structure='IPTS'
15 log_file = '/SNS/VIS/shared/VIS_team/VIS_logbook.csv' # needed only for weight=2
16 save_dir = '/SNS/VIS/shared/VIS_team/processed_data'  # needed only for save_flag=1 with post-processed files
17 #=========end of control block==========
18 #=========global parameters=============
19 scalex = 1.0; scaley = 1.0               # scaling parameters for x (energy transfer) and y (intensity)
20 shiftx = 0.0; shifty = 0.0                # shift along x and y (after scaling)
21 bin = '0.1,-0.001,5.4'      # binning parameters (meV)
22 smooth = 0                     # smooth parameter NPoints (0 for no smoothing)
23 unit = 'dSpacing'     # unit for output workspaces/files, ["dSpacing", "Momentum", "TOF", "Wavelength"]
24 #=========end of global parameters======
25 #=========data block==================
26 # the global parameters can be overwritten in the data block (redefined for a particular dataset)
27 # d.append( DataSet('16502-', 'b', bin='', smooth=, scalex=, scaley=, shiftx=, shifty=, tag=) )
28 d.append( DataSet('45762-', 'b') )
29 d.append( DataSet('48441-', 's') )
30 #-----------------------------
31 process_all(d,dict,file_structure,weight,root_dir,raw_subdir,red_subdir,log_file,bin,smooth,scalex,scaley,shiftx,shifty,unit,save_flag)
```

- Executing the above script will produce three workspaces: the background, sample, and sample with background subtracted. The diffraction datasets are labeled VIS_EED.
  o The same steps for background subtraction should be completed, as shown in the inelastic data reduction section above.
- The resulting diffraction pattern is split into 6 different banks corresponding to the 6 annular (90º) diffraction detectors.
- To save data in GSAS format, use the Algorithm *SaveGSS*.
- For Rietveld refinements, an instrument parameter file is needed for calibration with instrument specific values. It is best to consult the instrument staff for the correct file describing your experimental setup.
  o However, some instrument parameter files are located at /data/SNS/VIS/shared/VIS_users/eed_instprm.

LaB6 Diffraction