LDA DOS

Required Files

- compound/output/compound.int
- compound/output/compound.dos#ev

"compound" might be in shorthand
represents any number

Function

Read compound.int

Skip header information (the end of the header is determined by the string "NUMBER OF DOS CASES specified below")
Relevant data is expected to be in this format:
"WS#WS#WSElementWSDescription"
WS = White Space
# = any number
Element = name of an element
Description = equation (example: dz2)

Read .dos#ev file

First 3 rows are header information
First column is energy level (x-axis in plots)
The columns of .dos#ev going left to right correspond with the rows of .int file going top to bottom

Example:
In the int file,
a
b
c
In the .dos#ev file,
freq/energy a b c

Append each column of .dos#ev to a data object
Data object records plot data (numbers), index (column number in .dos#ev file or row number in .int file), equation (description of data)

If there are n data columns (not total columns) in .dos1ev, then the first column of data in .dos2ev will represent index (n+1).

Output

Visual plot generated from data
Searches for specific data sets are based on index and equation
X,Y axis can be modified
Grid can be applied
Data also is presented in files
Data files exist for one week from the time of creation
name of file: ldadosEQUATION.txt

format of data file:
1st column: x-data
2nd column: y-data