Hyper-EMG
Fitting Peak Shapes and Determining Mass values

Begin Code

Get User Inputs

- Txt file paths
- Initial centroid guesses
- Number of desired tails
- Initial parameter guesses

Begin Fitting Peak Shape Calibrant

Load Peak Shape Calibrant File Data

- Get normalization factor
- Assign uncertainty to data - sqrt(N+1)
- Normalize data and error

Fit a Gaussian to Data

- Set Initial centroid guess as maximum y-val in file
- Fit Gaussian to data
- Plot data and new Gaussian fit

Fit a Hyper EMG to Peak Shape Data

- Set Initial centroid and stdev guess as those found from the Gaussian fit
- Fit (n,m) Hyper EMG
- Plot fit on same graph as Gaussian

Save and Display Hyper EMG Fit Results

Plot Residuals Graph

- Subtract fit from original data
- Force all y values within the FWHM to zero (to focus on tails)

Begin Applying Peak Shape to Ion of Interest Data Sets (Doublet or Triplet)

Load I or Interest File Data

- Assign uncertainty to data - sqrt(N+1)

Fit Peakshape to Spectrum

- Use user inputed initial centroid guesses
- Use peak parameters found from peak shape calibration

Display Fit and Optimized Parameters

Also Displays:

- The individual peaks that make up the sum fit
- Counts in each individual peak
- The separations between each peak in the spectrum
- Reduced Chi squared value

Plot Residuals Graph

- Subtract fit from original data
- Force all y values within the FWHM to zero (to focus on tails)

Find Fit Uncertainty
Determining Statistical and Peak Shape Uncertainty

Begin Code

Get User Inputs

- Txt file paths
- Optimized parameters found in Hyper EMG code
- Number of tails used in peak shape calibration

Load all Data Files Individualy

- Assign uncertainty to data - sqrt(N+1)
- Normalize peak shape calibrant peak and corresponding errors

Get Statistical uncertainty for each individdual peak

- Find counts in each individual peak

$$\frac{0.53 * 2.355 * StDev}{(counts)^{0.5}}$$

Save All Value for Future Displaying

Loop Start

For a Given Parameter: (all other parameters fixed)

Was the parameter optimized/ used in the Hyper-EGM fit?

Yes / No

Next

Create parameter upper and lower limits:

- UpperParam = parameter + error
- LowerParam = parameter + error

Is this parameter relevant to the peak shape calibrant fit?

Yes / No

Peak Fit to Determine New Centroid:

UpperParam = parameter+ error
or
LowerParam = parameter + error

Is this parameter relevant to the Doublet peak fit?

Yes / No

Peak Fit to Determine New Centroid:

Upper = parameter+ error
or
Lower = parameter + error

Is this parameter relevant to the Triplet peak fit?

Yes / No

Peak fit to determine new centroids:

Upper = parameter+ error
or
Lower = parameter + error

Pass

Pass

Done all parameters?

No / Yes

Quadraticaly Add All Deviations for Each Individual Fit:

Total deviation=$((dev1)^2+(dev2)^2...)^{0.5}$

Determine UpperParam's and LowerParam's Deviation from the Original Value for Each Fit Individually:

$$\frac{|\ UpperParam - original\ | + |\ LowerParam - original\ |}{2}$$

Print All Uncertainties