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Basics of Data Processing

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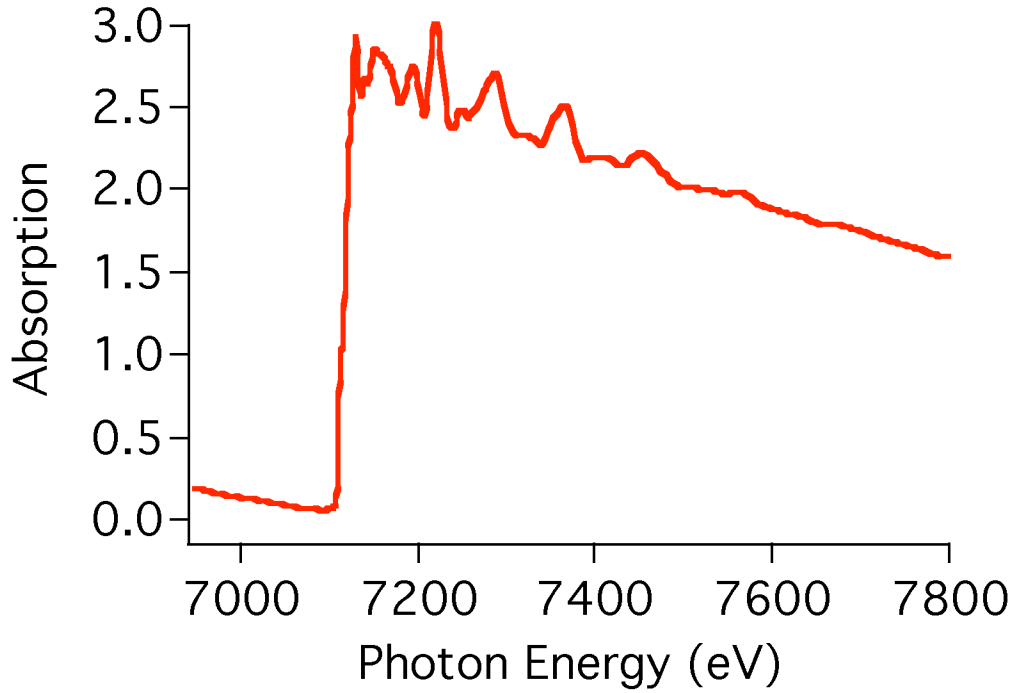
Data Processing Overview

Transmission: $\mu(E) = \ln(I_o/I_t)$

Fluorescence: $\mu(E) = I_f/I_o$



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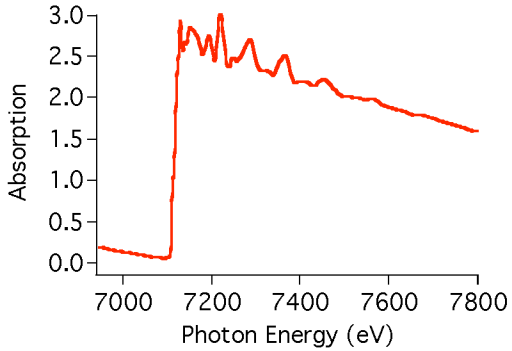
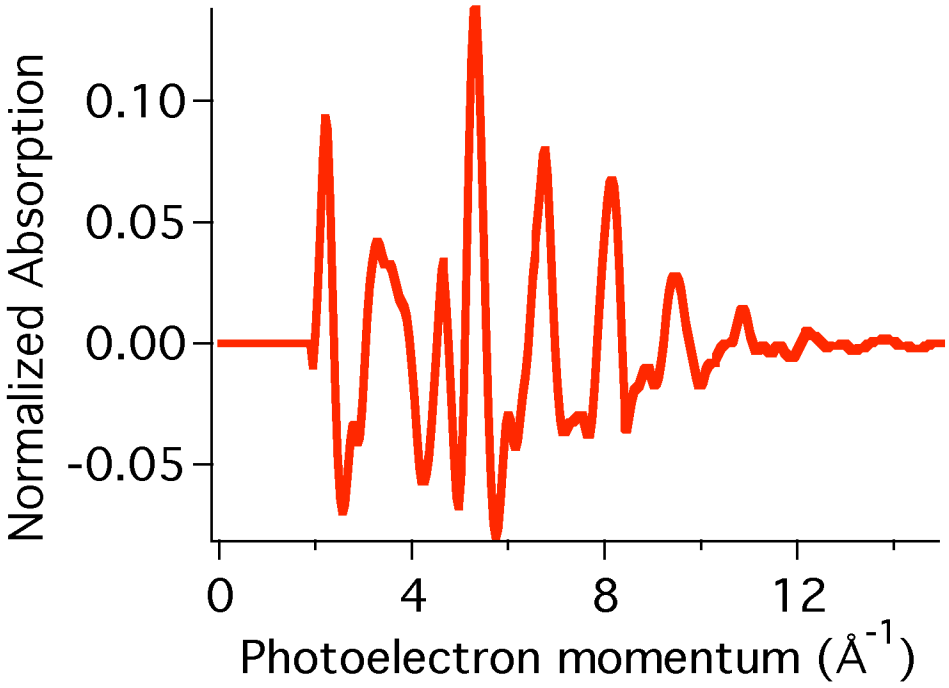
Data Processing Overview



$\chi(k) = [\mu(E) - \mu_0(E)]/\Delta\mu(E_0)$



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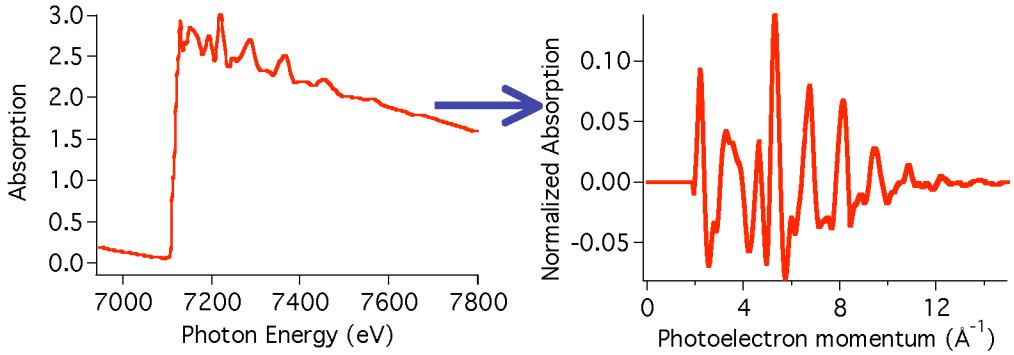
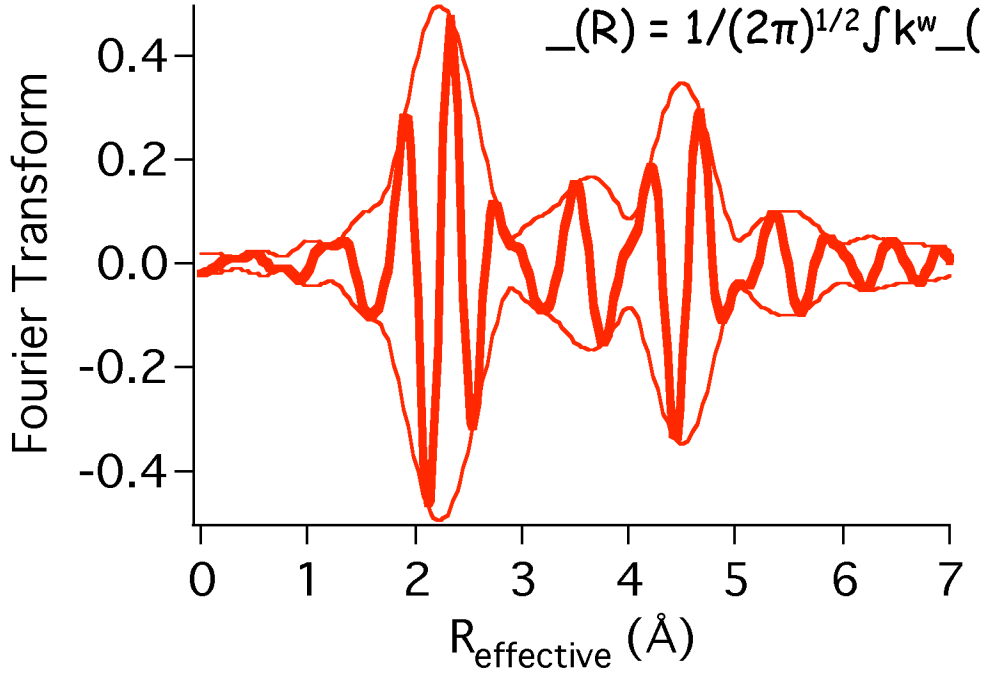
Data Processing Overview



$$\chi(R) = 1/(2\pi)^{1/2} \int k^{w} \chi(k) W(k) e^{i2kR} dk$$



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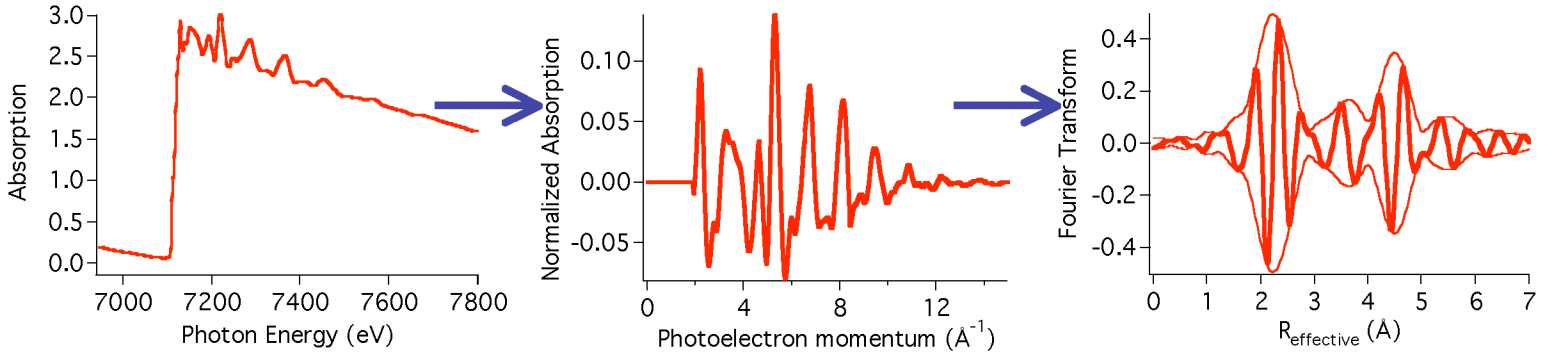
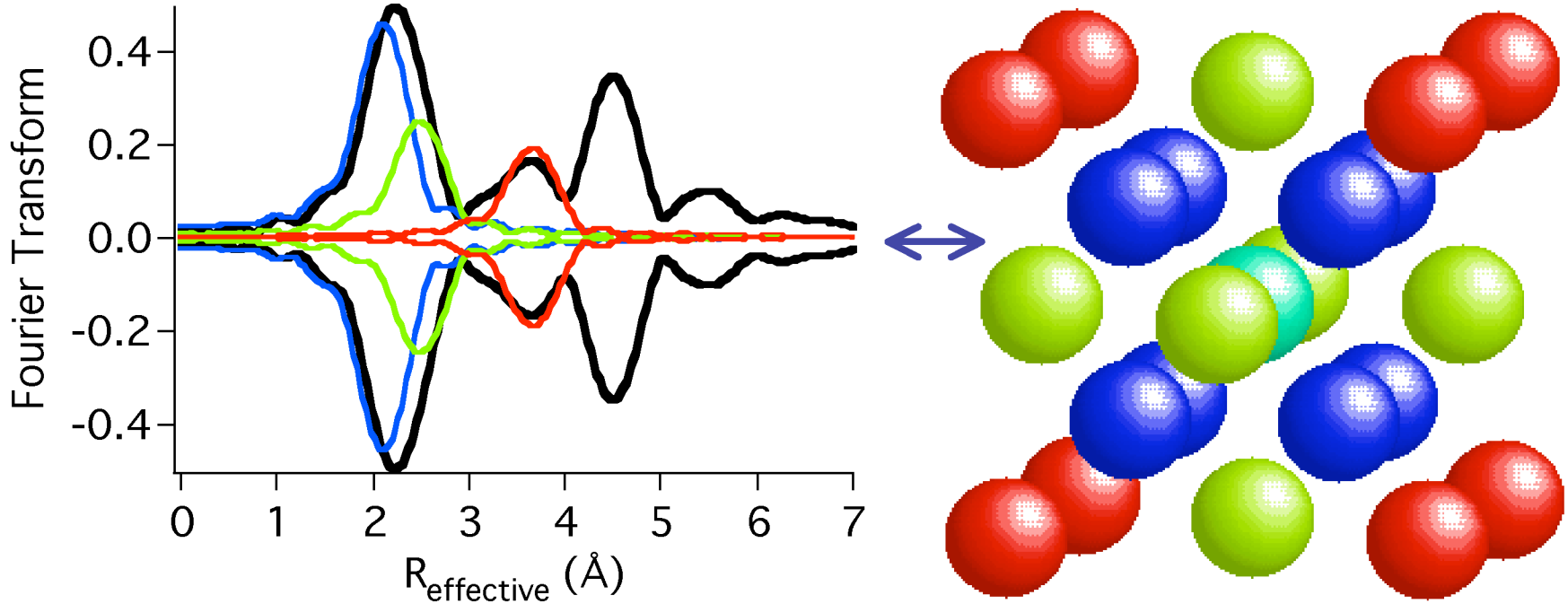
Data Processing Overview





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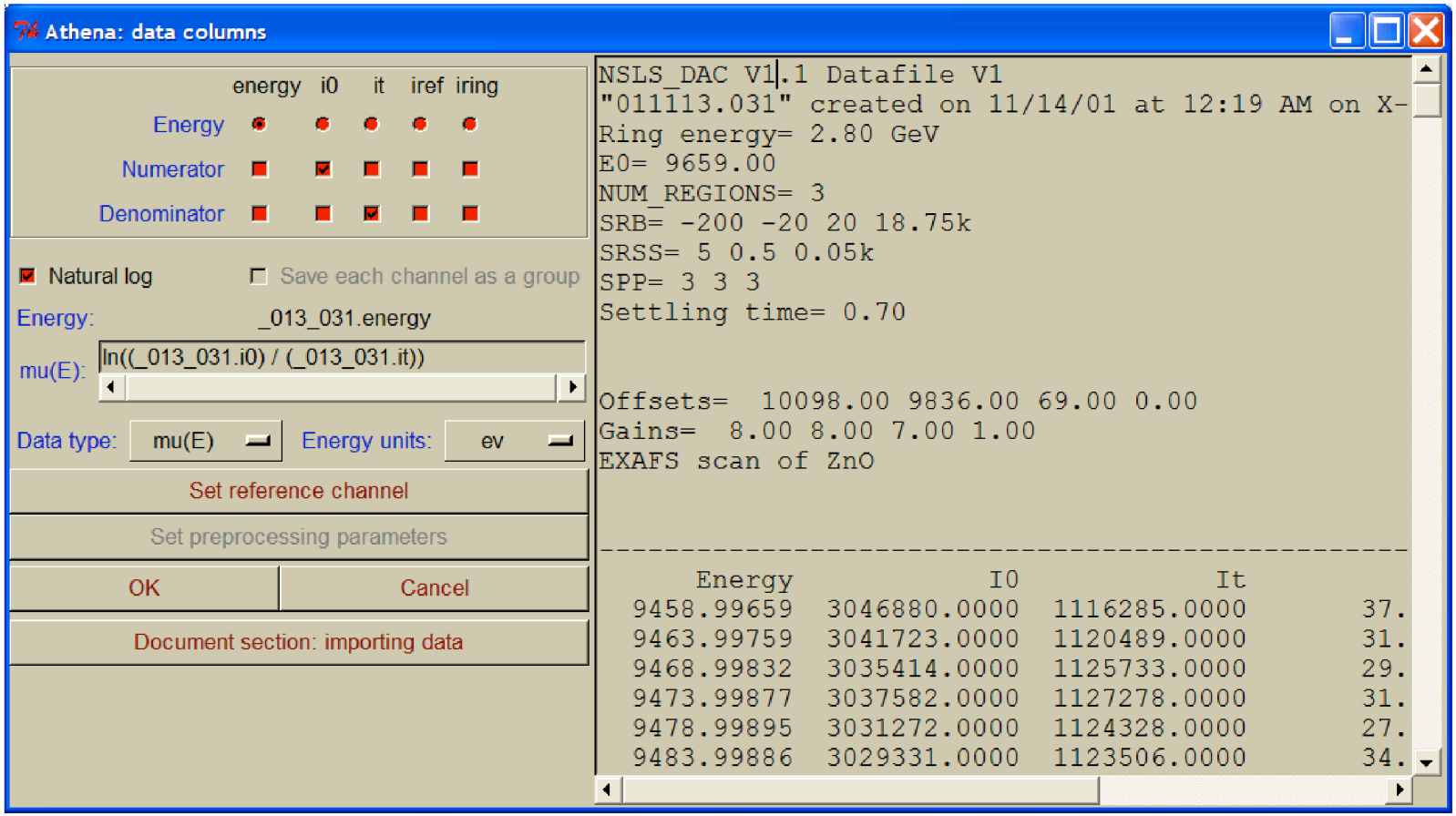
Importing Raw Data in Athena



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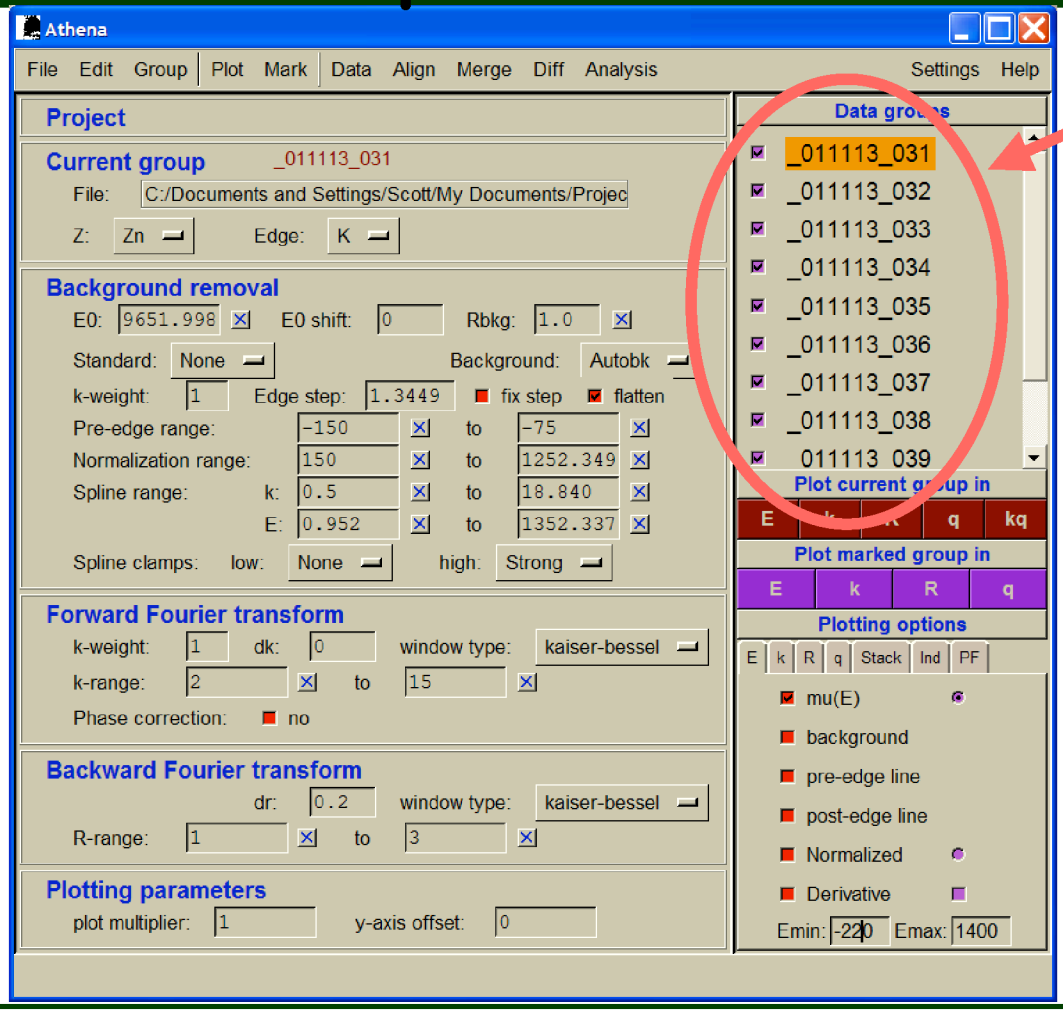
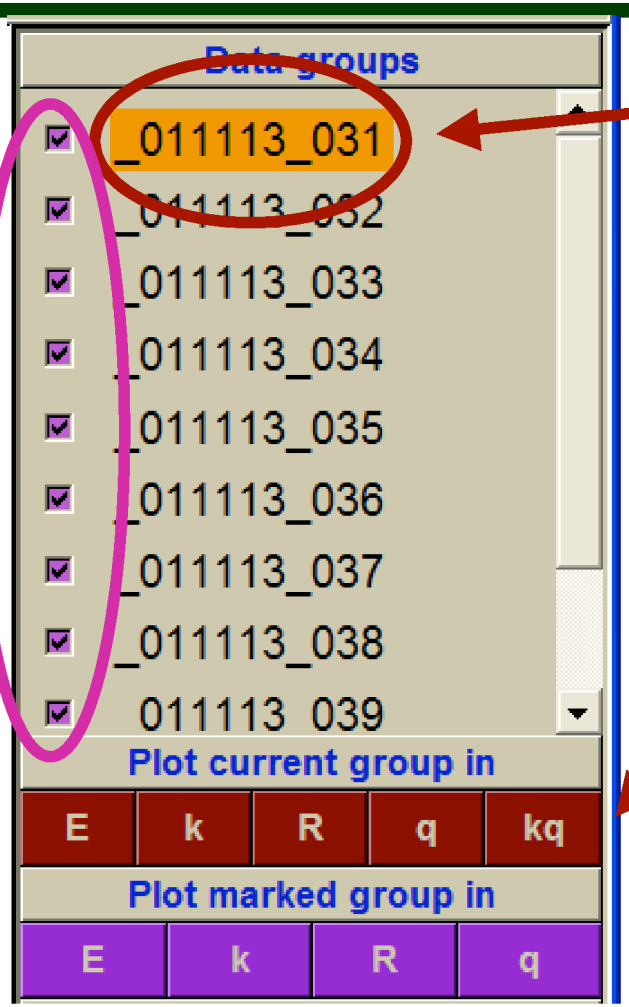
Groups in Athena



"Groups" include individual scans

"Marked" and "Current" Groups



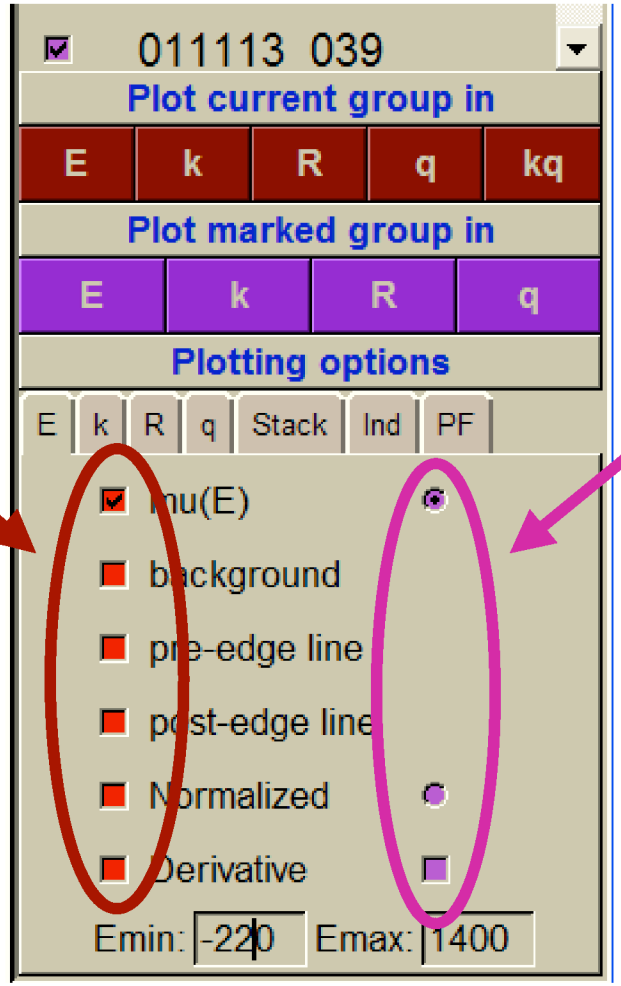
Checks indicate "marked" groups

This is the "current" group

Note that these buttons plot the current group

These buttons plot all the marked groups

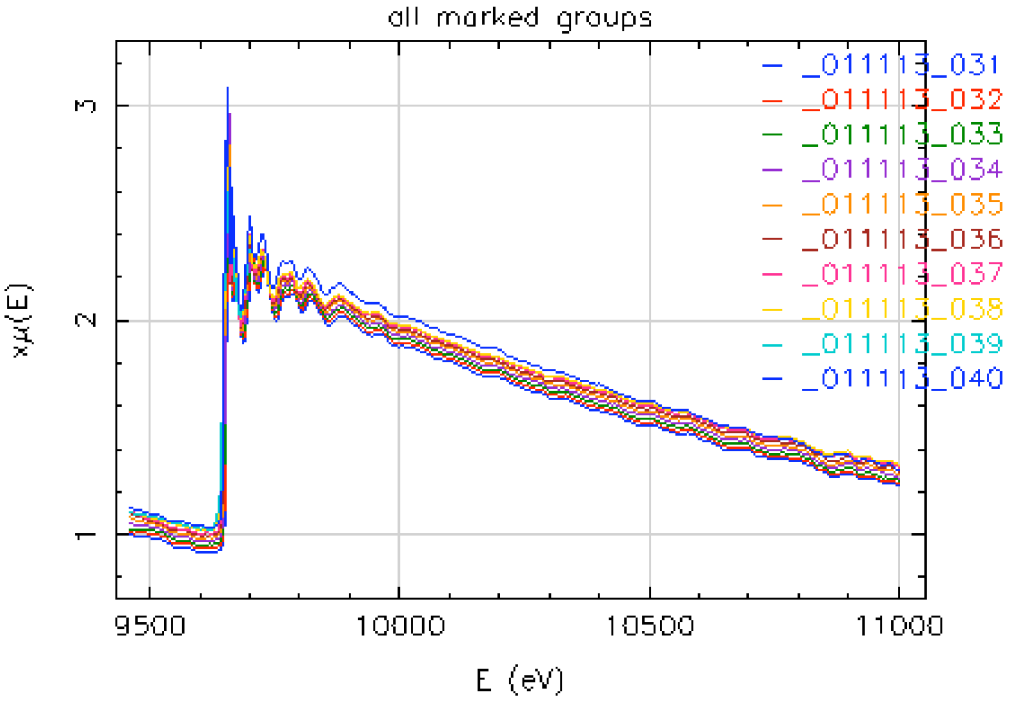
"Marked" and "Current" Groups



These options affect plots of the current group

These options affect plots of all marked groups

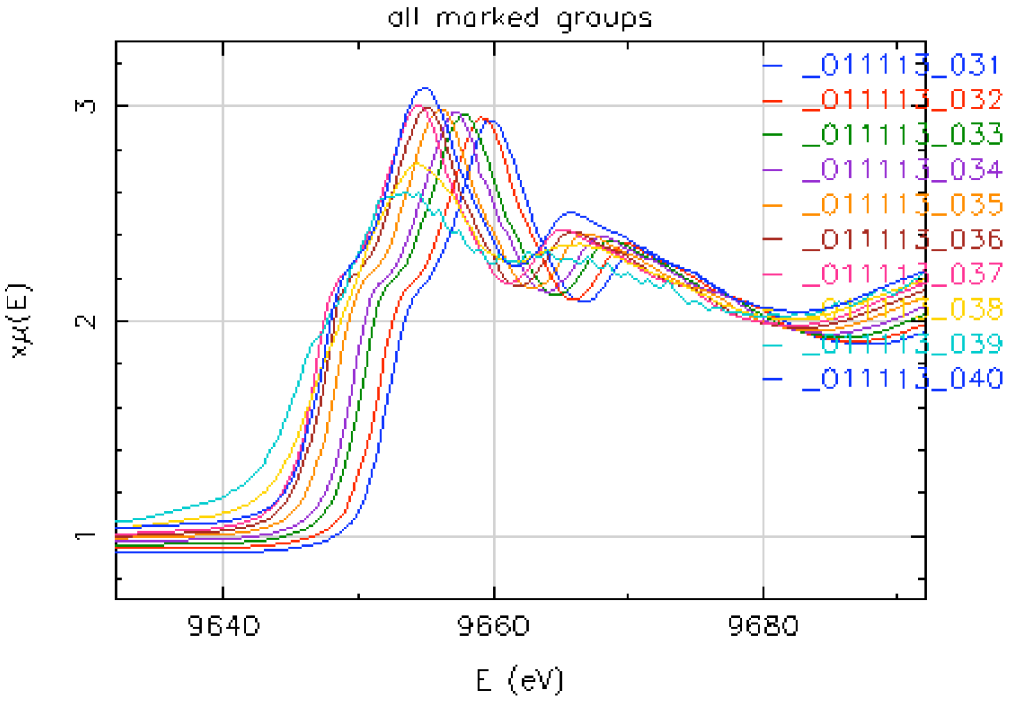
Compare Scans



Vertical translation between scans will not affect EXAFS

But a closer look…

Compare Scans

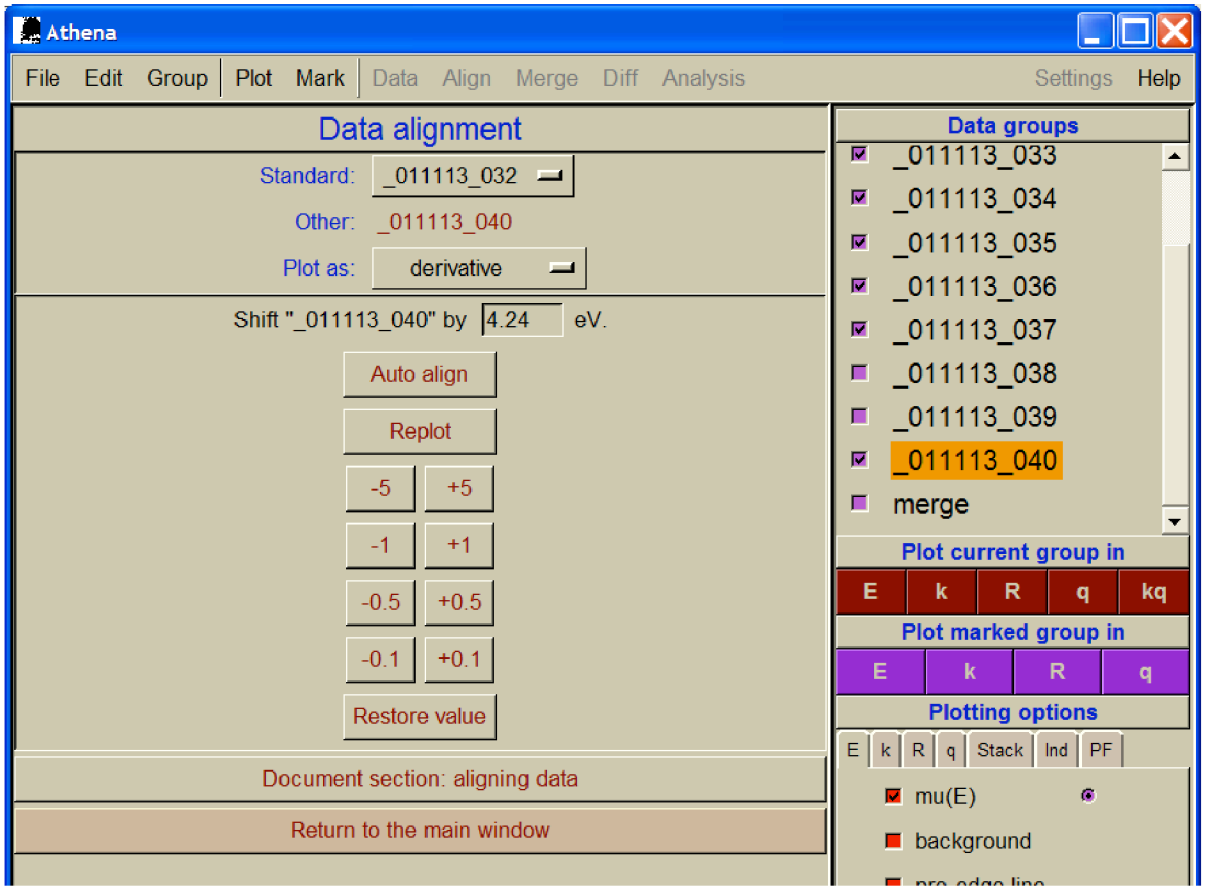


…reveals other problems.

Energy calibration appears to have drifted

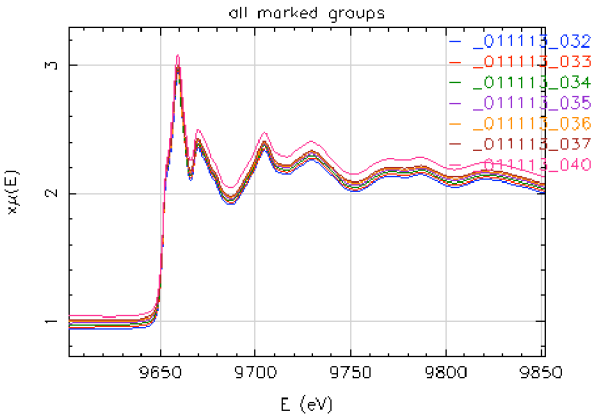
Scans 38 and 39 appear inconsistent with the rest

Alignment in Athena



Under the "align" menu, you can have Athena attempt to shift scans for you, or you can do it "by hand"

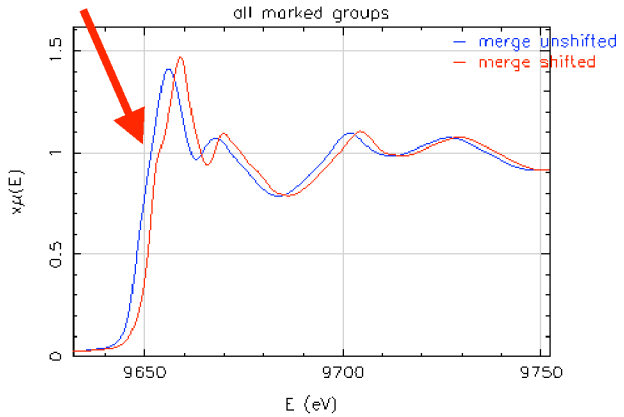
Alignment Matters



The scans are now aligned

If we had not aligned them, the average would show considerable differences:

Note missing shoulder on unaligned version



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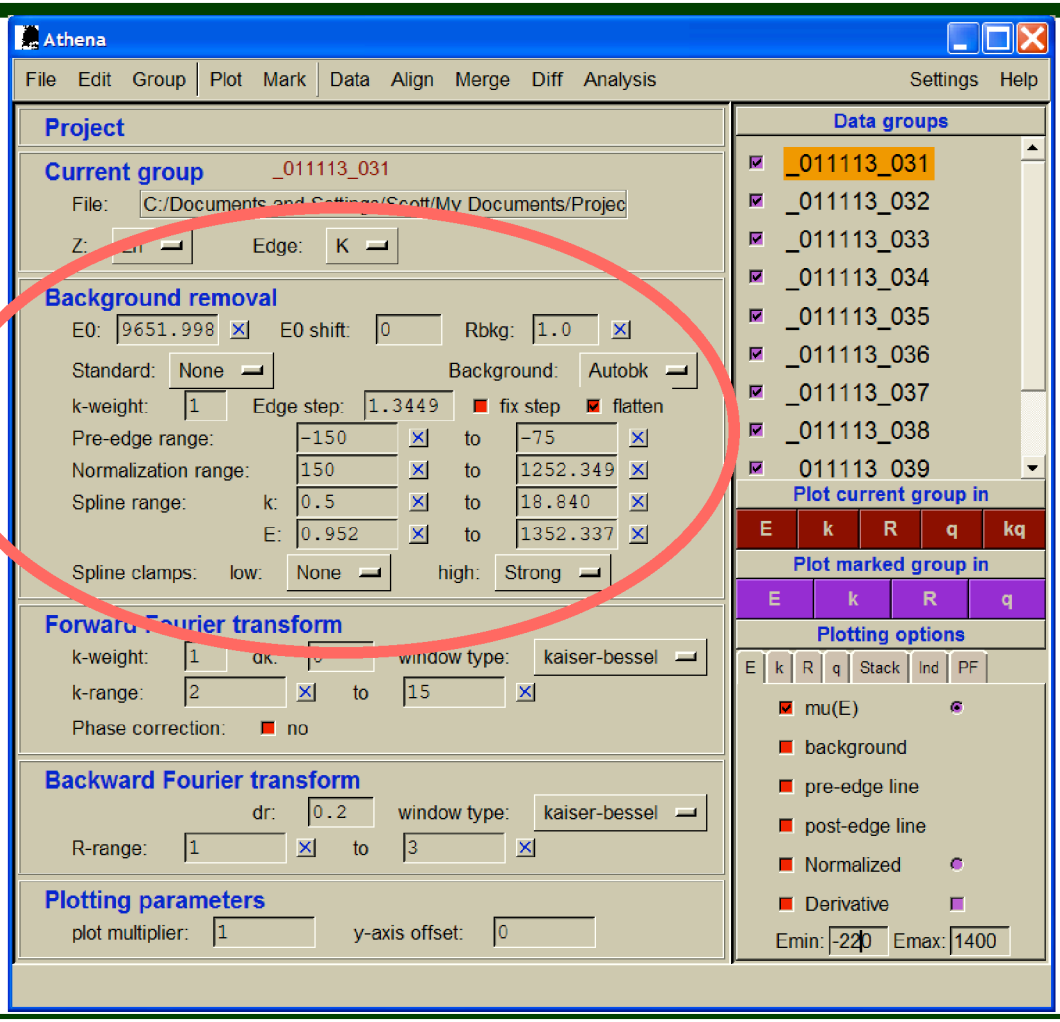
Background Removal in Athena

This information applies to the *current* scan

Right clicking brings up a menu that lets you apply these settings to all scans, or to all *marked* scans



alignment is very important

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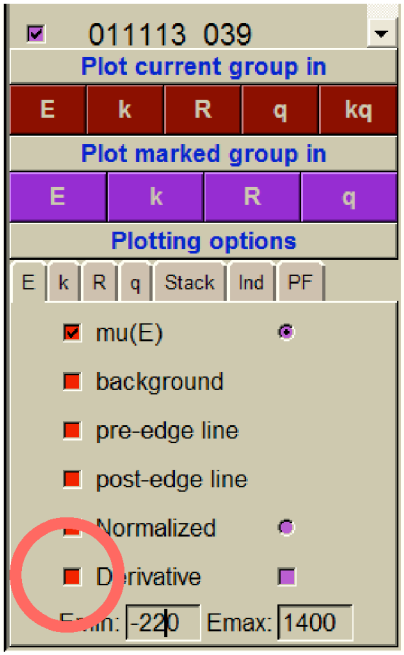
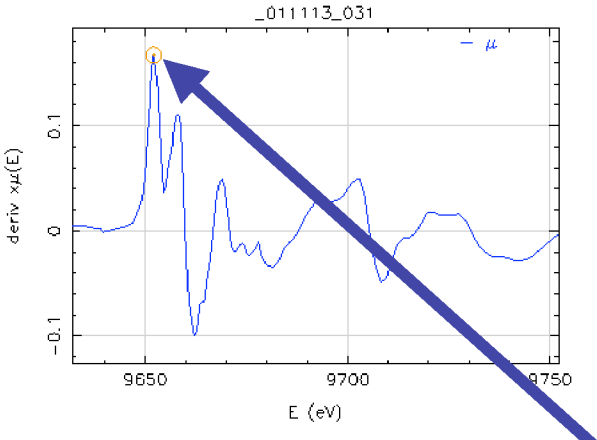
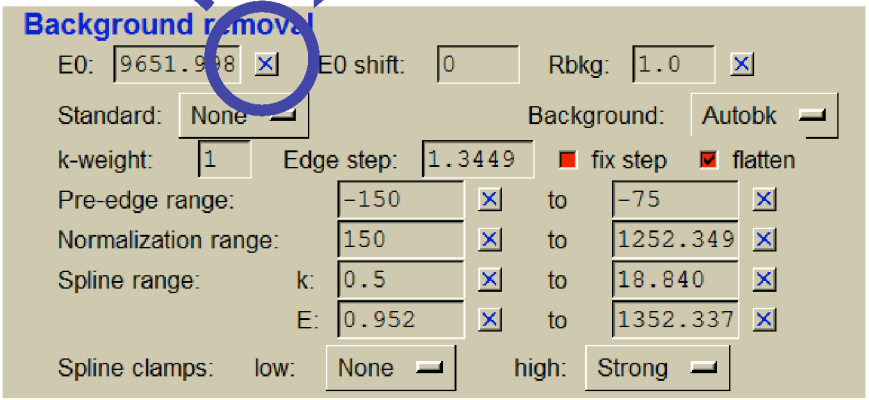
Choosing E_o in Athena



Click here to see a plot of the derivative spectrum

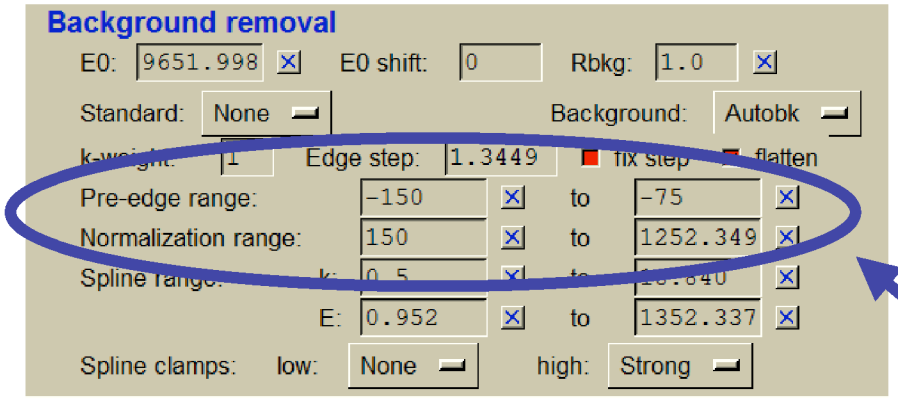


Choose E_o at first peak in the derivative spectrum



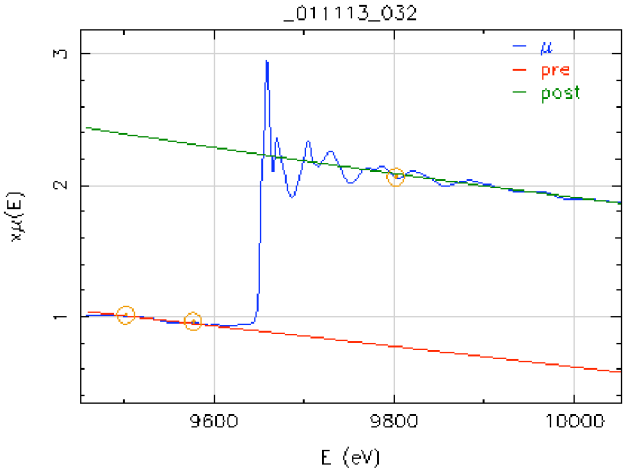
Choosing E_o carefully is of low importance for EXAFS, as long as it is done consistently for all scans

Normalizing in Athena

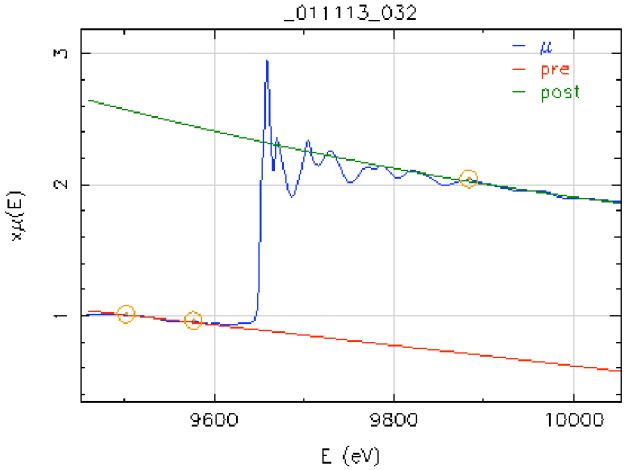


Choose pre-edge and normalization ranges

Good and Bad Normalization

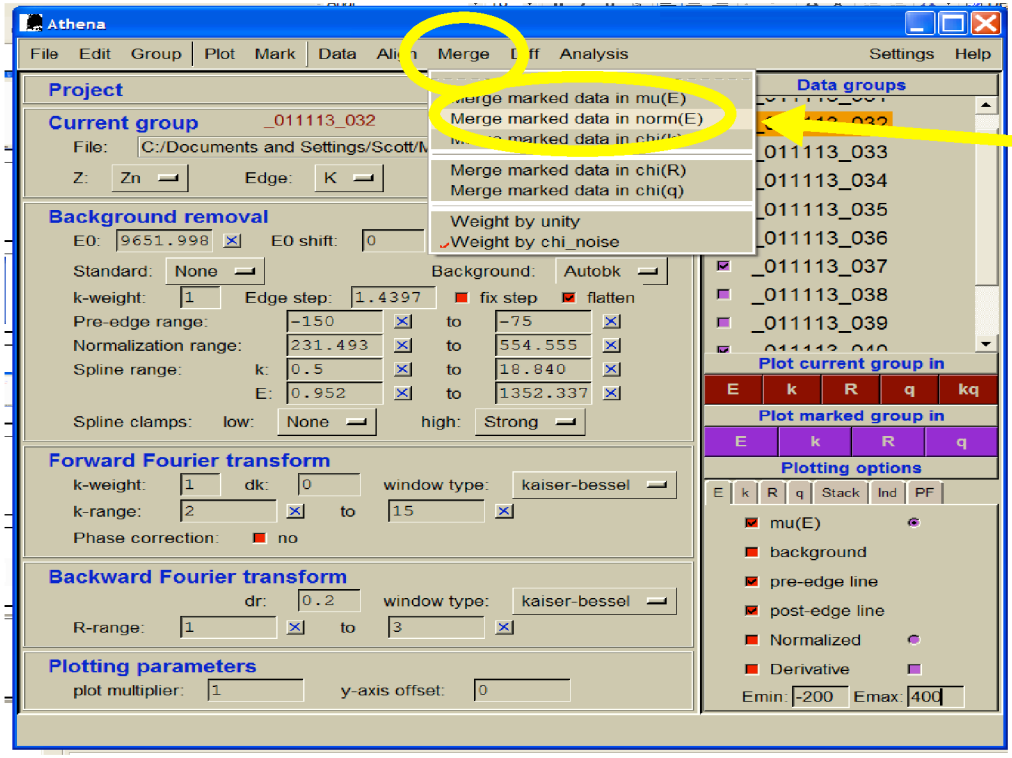


These pre- and post-edge lines look OK

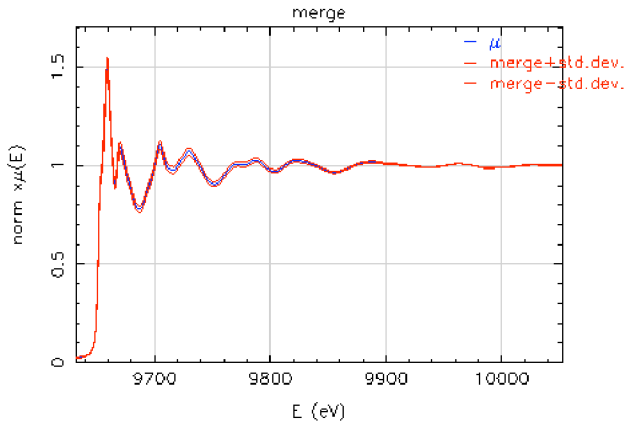


This post-edge line goes too high near edge

Merging Data in Athena



Merge aligned and normalized scans here



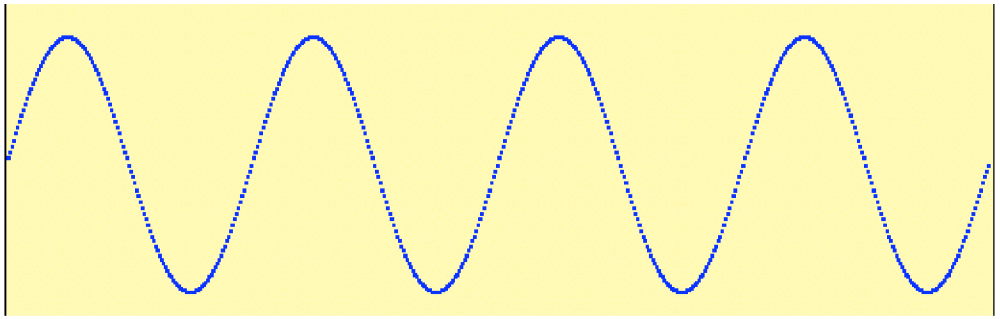
Normalization may be very important in some cases, such as determining coordination number when you think you know S_o^2, but if you are fitting S_o^2 it is relatively unimportant

Graphs on the following series of slides obtained from:

http://members.nuvox.net/~on.jwclymer/graphs/fourier.html

Fourier Transforms

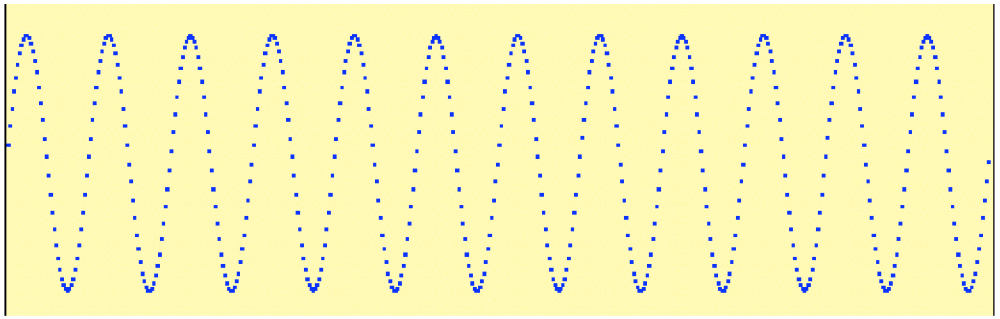
A sin function…



…has a Fourier transform which is in theory a delta function at the frequency of the sine wave

Fourier Transforms

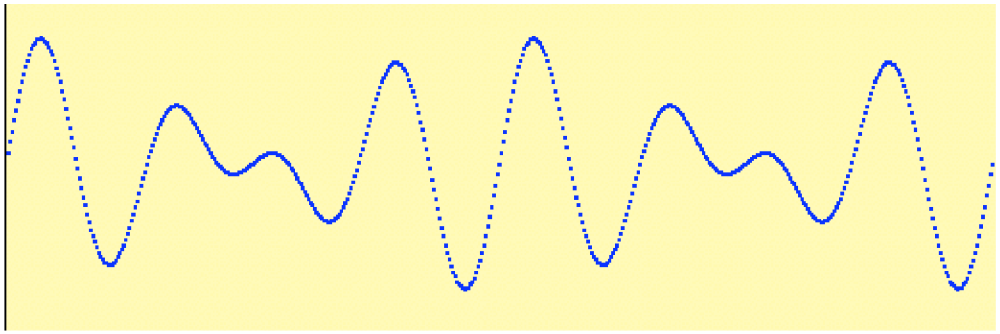
A higher frequency…



…shifts further right in the Fourier transform

Fourier Transforms

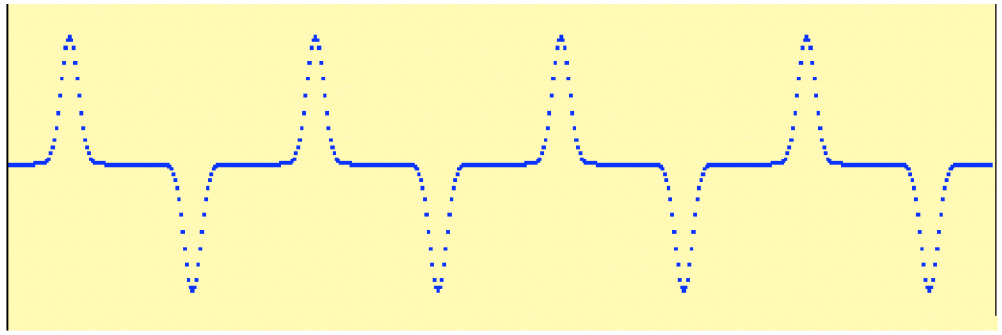
A more complicated pattern…



…is made up of more than one frequency

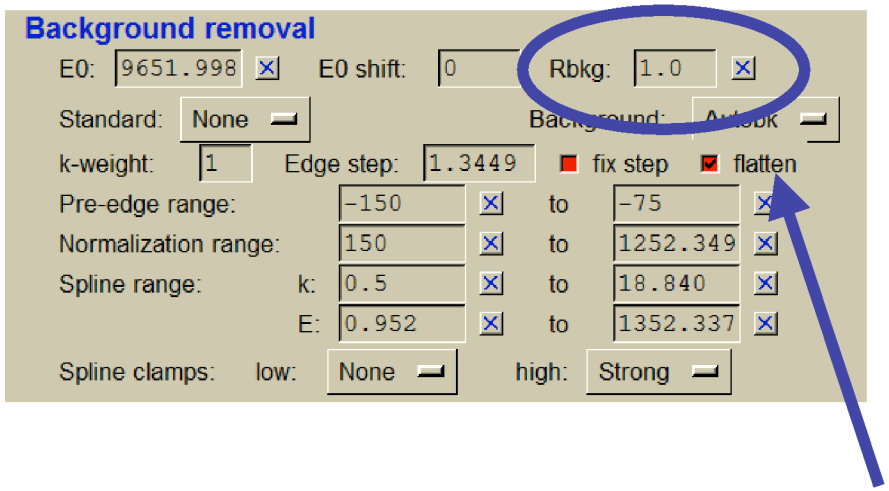
Fourier Transforms

A pattern with sharp features…



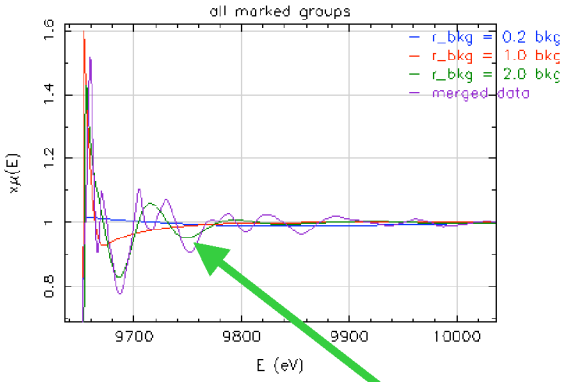
Has extra components higher in Fourier space…

R_{bkg}

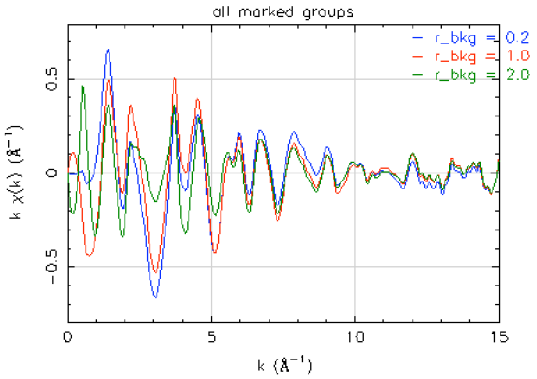


R_{bkg} controls how far up in the Fourier transform the background will try to suppress; i.e. how "wiggly" the background can be

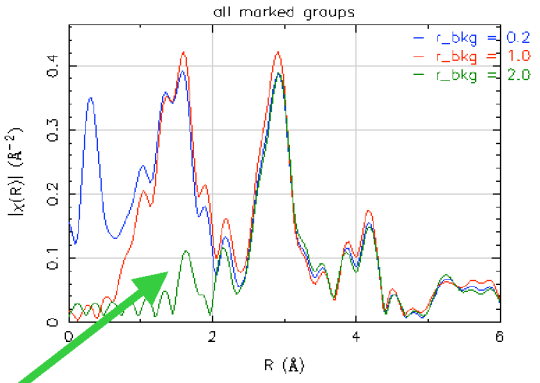
R_{bkg}



Energy plot



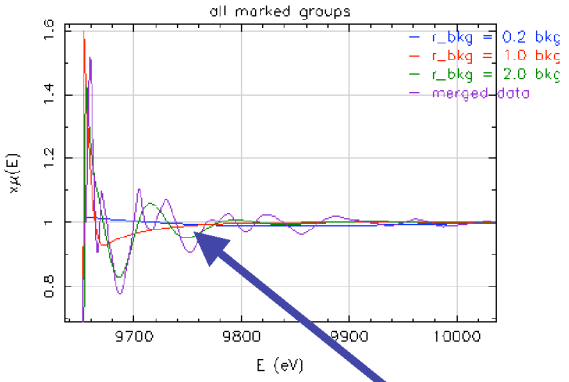
k-space plot



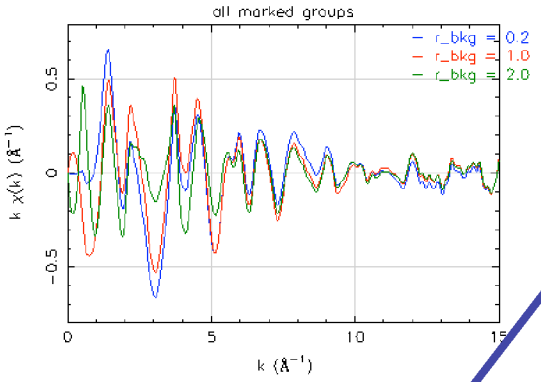
Magnitude of Fourier transform

R_{bkg} of 2.0 _ wiggles too much in energy space and thus kills off low-R peak in Fourier transform

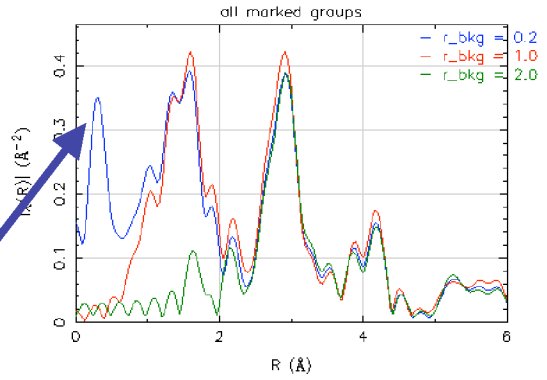
R_{bkg}



Energy plot



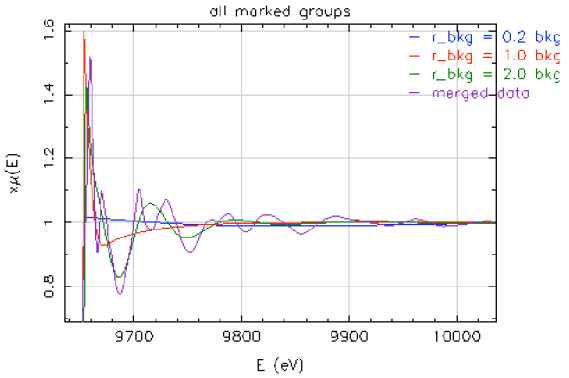
k-space plot



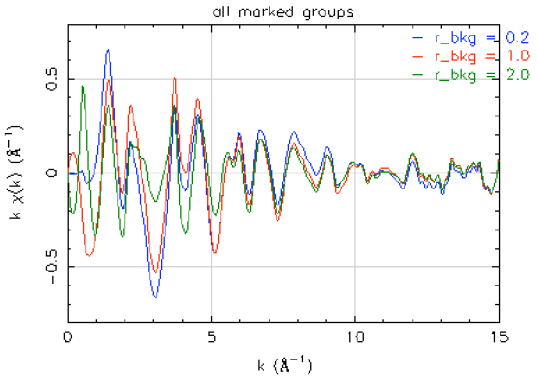
Magnitude of Fourier transform

R_{bkg} of 0.2 Å "misses" in energy space and thus introduces spurious low-R peak in Fourier transform

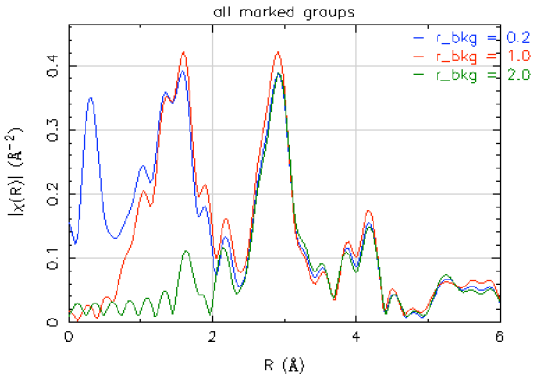
R_{bkg}



Energy plot



k-space plot



Magnitude of Fourier transform

R_{bkg} of 1.0 Å is OK!

R_{bkg} is fairly important

Ideally, small changes in R_{bkg} should not significantly change the parameters you find via your fits

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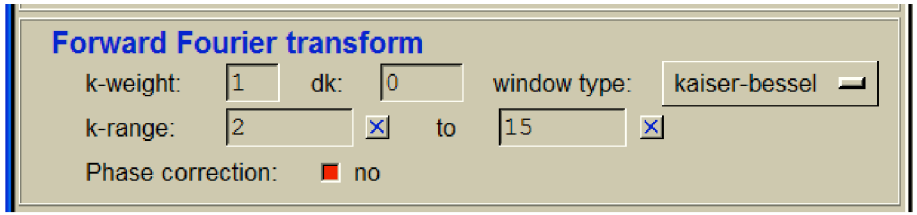
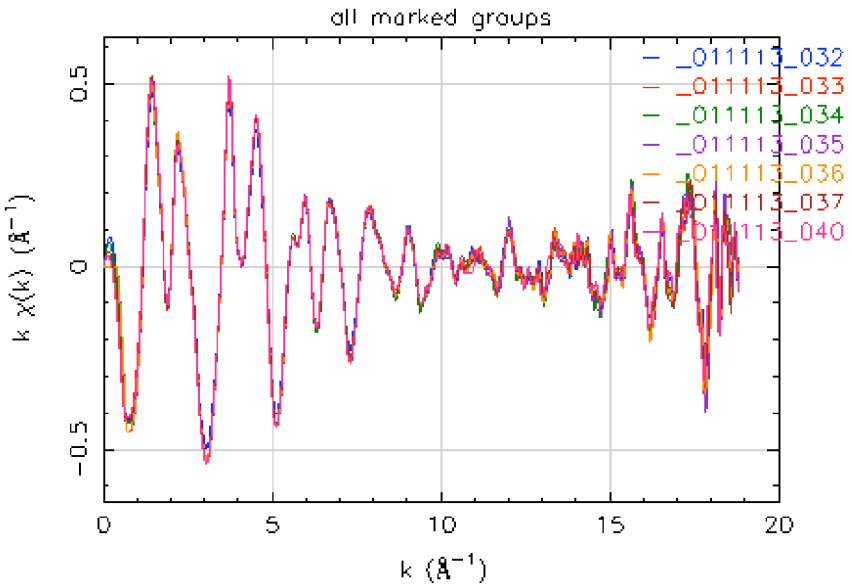
Fourier Transforms in Athena



Choosing k_{max}



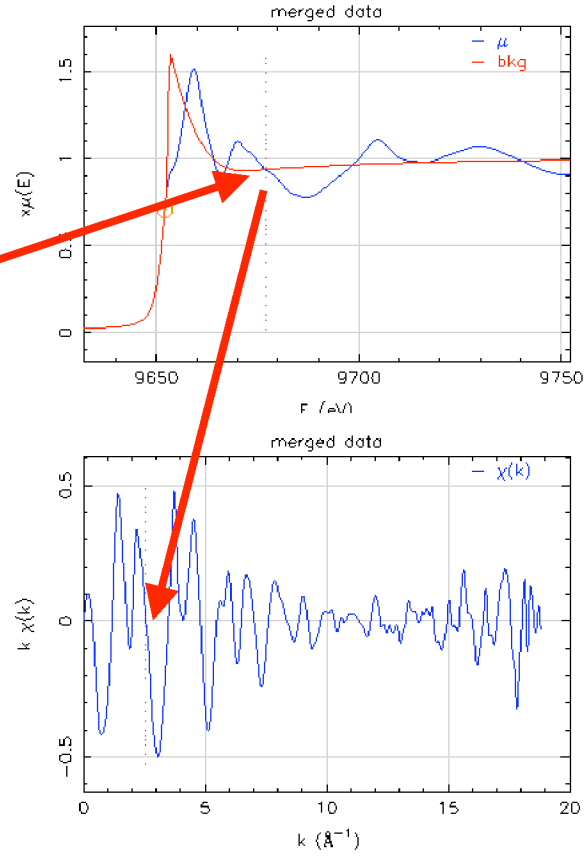
This data appears consistent for all scans. If there is trouble at high-*k*, it is systematic and reproducible.

Choice of k_{max} should be of low importance

Ideally, small changes in choice of k_{max} should not change parameters you find via your fits

Choosing k_{min}

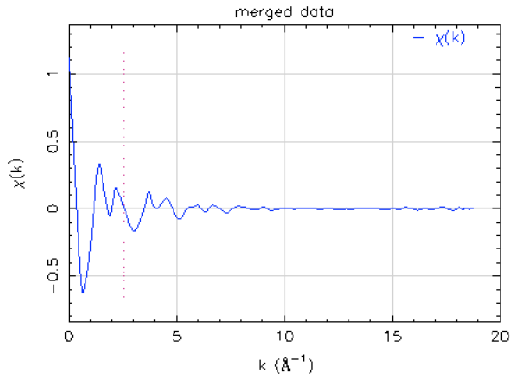
Choose k_{min} where background stops being strongly dependent on small changes in background parameters



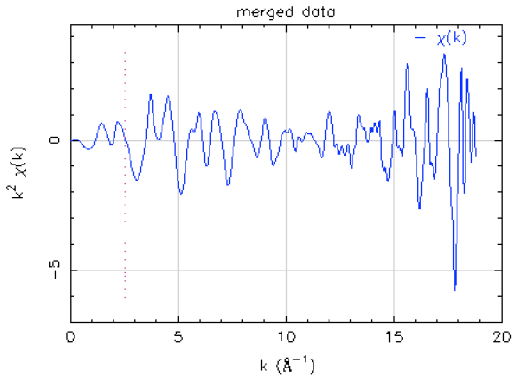
Choice of k_{min} *should* be of low importance

Ideally, small changes in choice of k_{min} should not change parameters you find via your fits. In practice, fit is often more sensitive to k_{min} than k_{max}

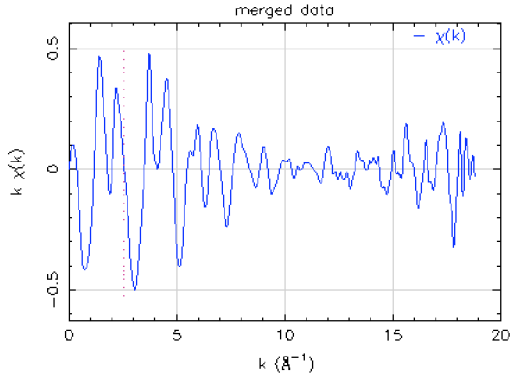
k-weight



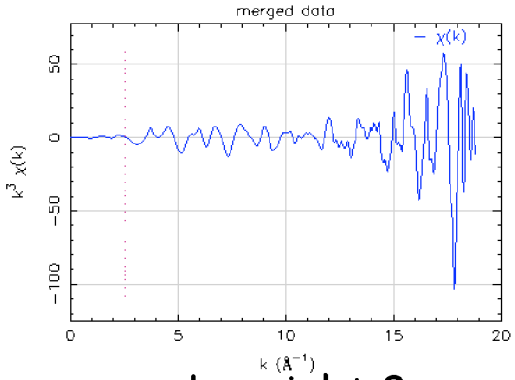
Unweighted



k-weight 2



k-weight 1



k-weight 3

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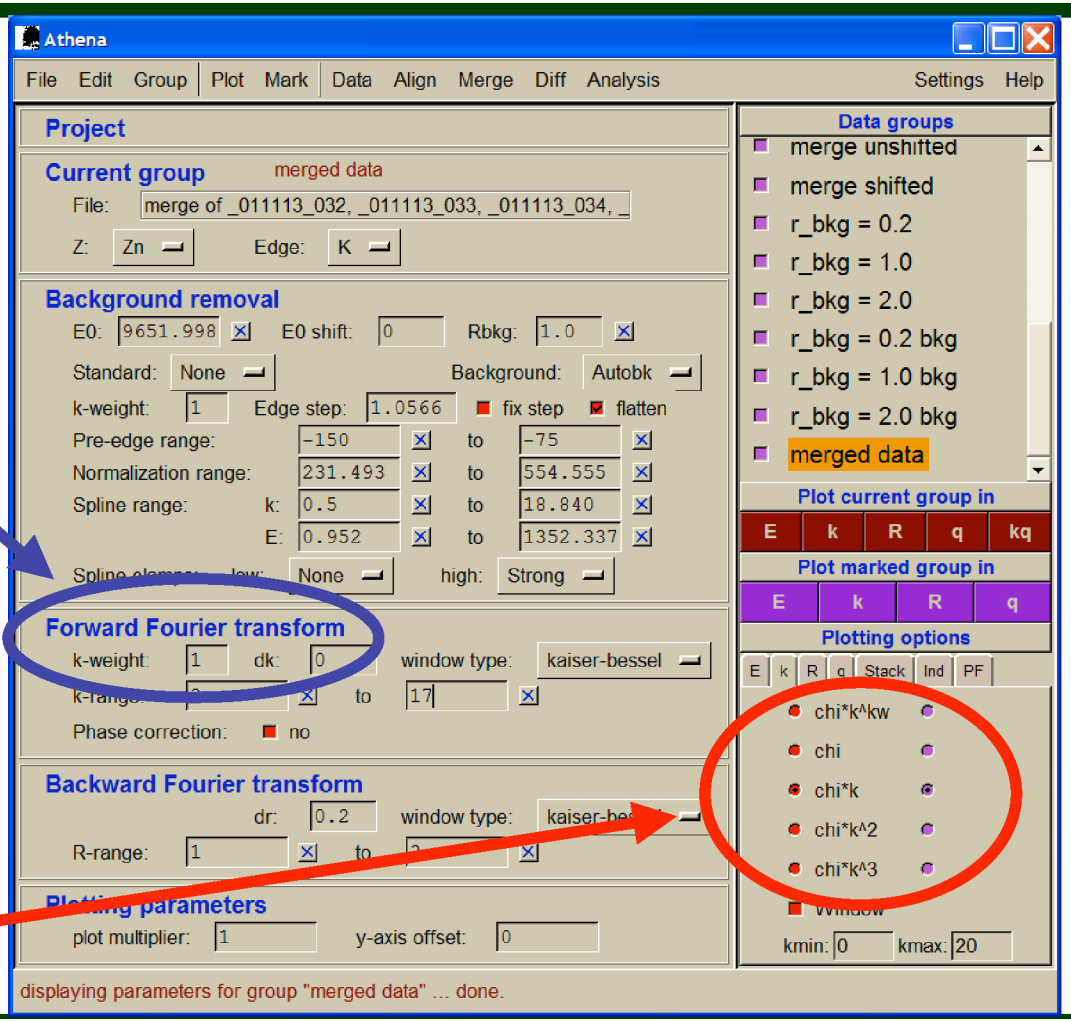
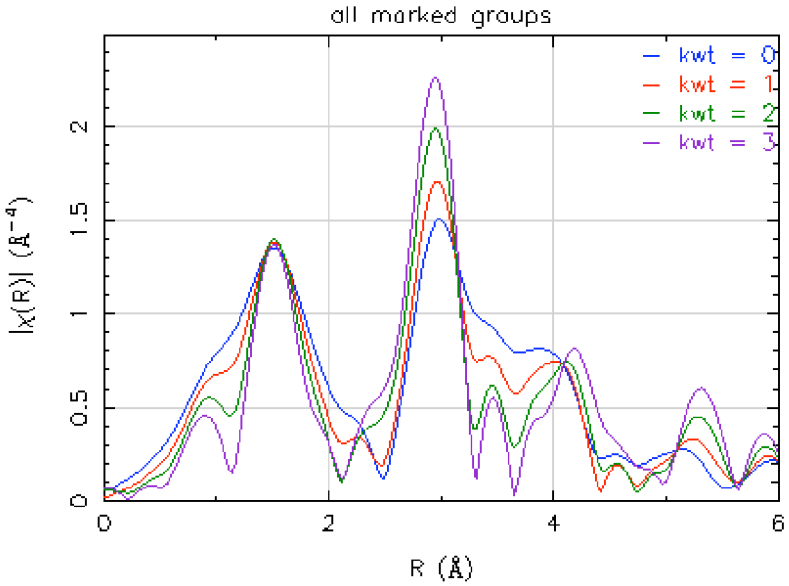
Athena Reminder!

This affects the Fourier transform

This affects the k-space plot



Effect of k-weight on Fourier Transform



k-weight *should* be of low importance

Ideally, different k-weights should not change parameters you find via your fits.

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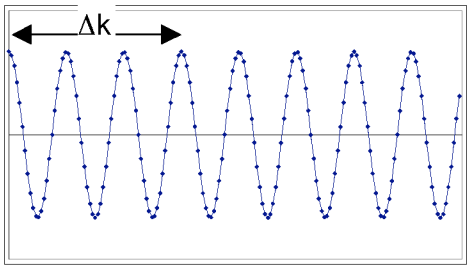
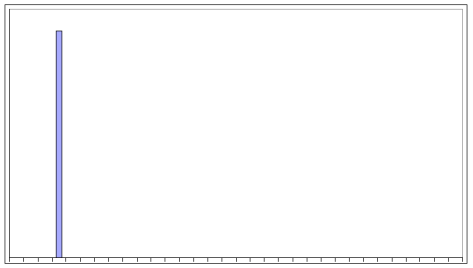
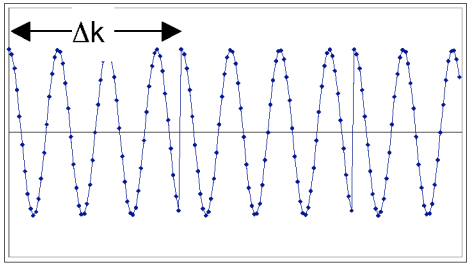
Fourier Transform Artifacts

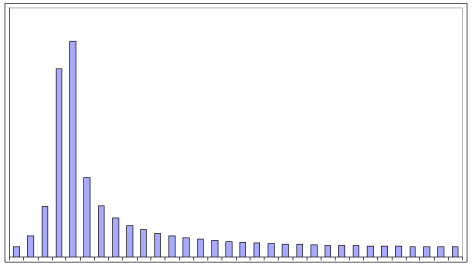
Lucky function



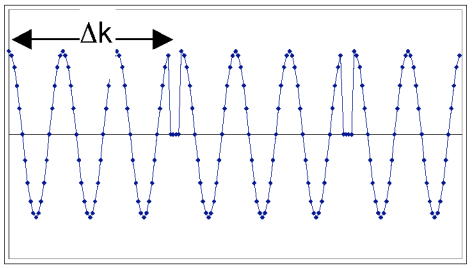


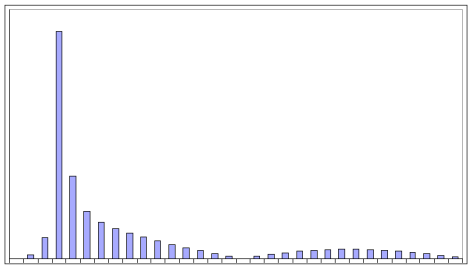
Unlucky function



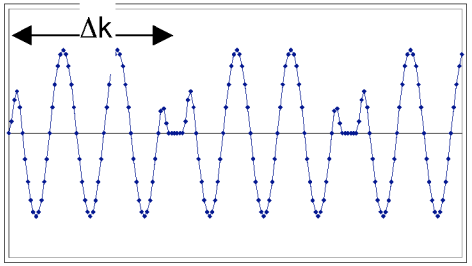


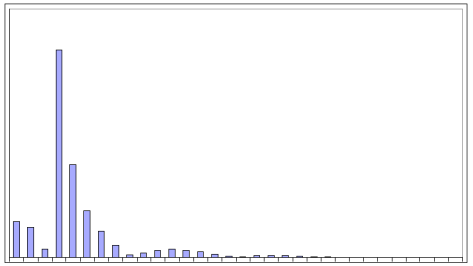
Padded with zeroes



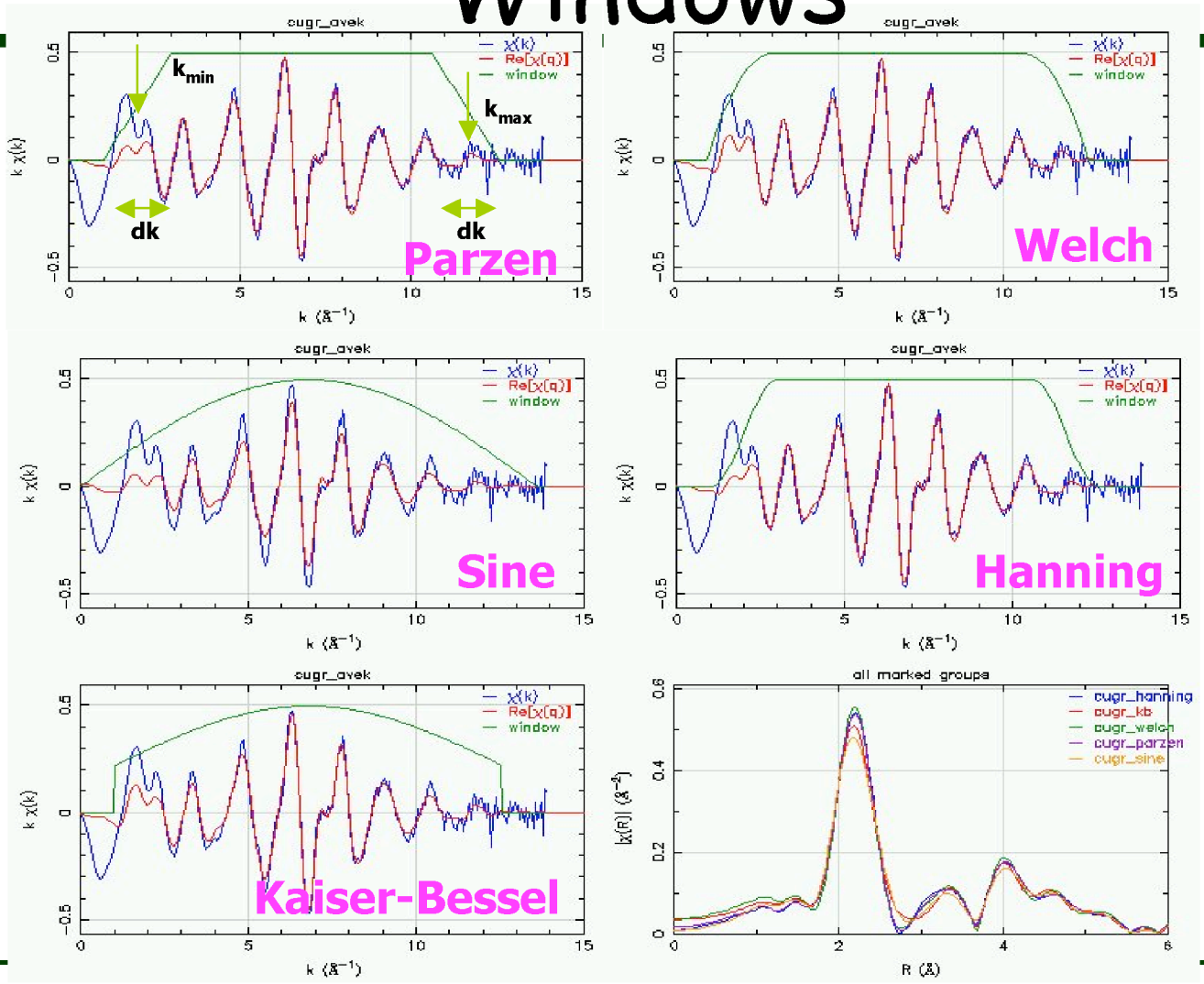


Windowed





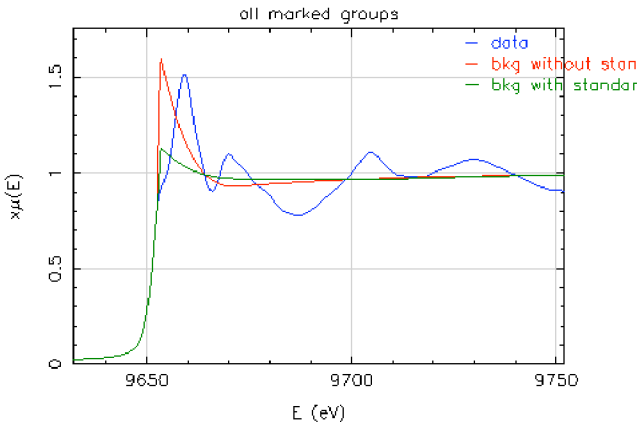
Windows

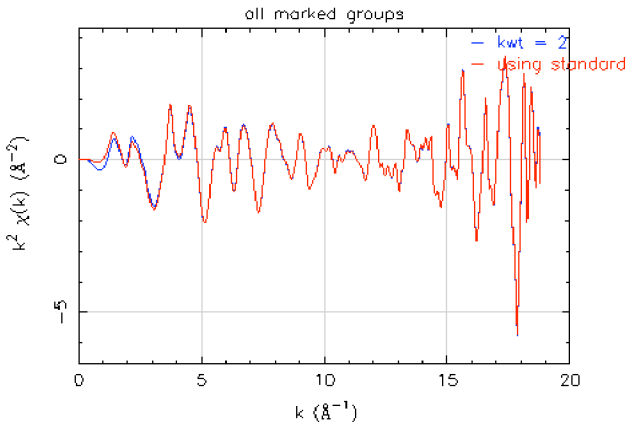

cugr_avek
χ(k)
Re[χ(q)]
window
k χ(k)
k (Å⁻¹)
k_min
k_max
dk
dk
Parzen
Welch
Sine
Hanning
Kaiser-Bessel
all marked groups
cugr_hanning
cugr_kb
cugr_welch
cugr_parzen
cugr_sine
|χ(R)| (Å⁻³)
R (Å)

Choice of window is of low importance

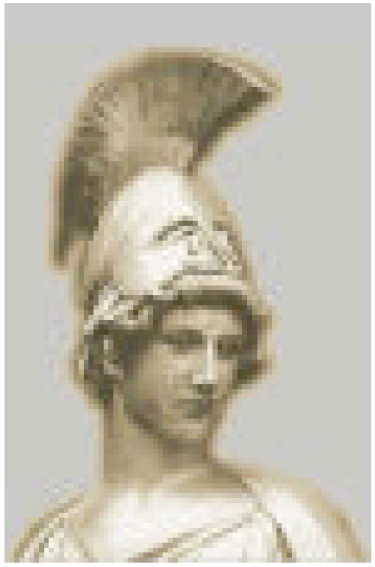
and should not change parameters you find via your fits.

Using a Standard for Background Subtraction





Using a standard for background subtraction may be of some importance, but the precise choice of standard should not be



Happy Processing!