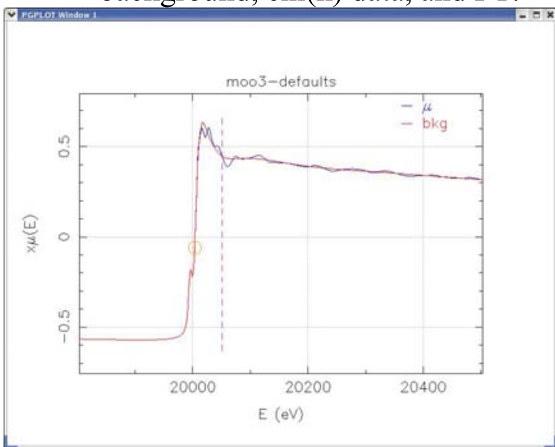
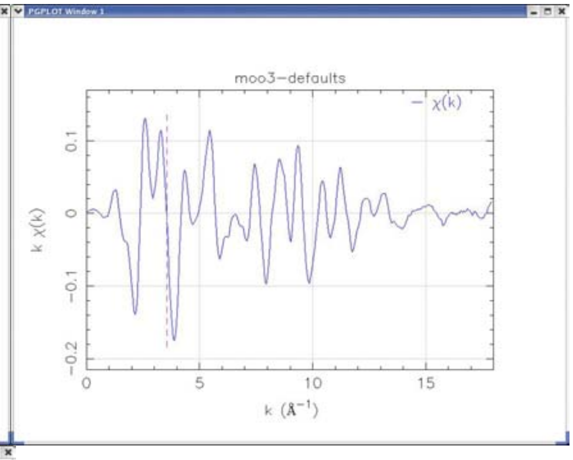
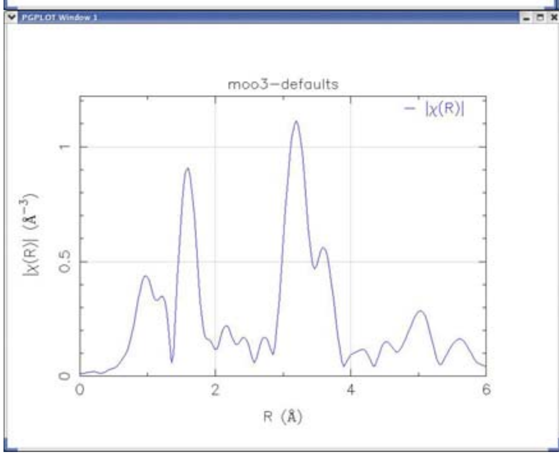
This tutorial is to show step by step process for removing a "tough" background. This tutorial uses MoO_3 which has a split close oxygen first shell and a lot of structure in the "XANES" region of the EXAFS data. This tutorial uses the theoretical chi(k) spectra to determine the shape of the background function through the "XANES" region of the absorption edge. At the end of the tutorial I give an example of how a similar background can be determined without the use of a theory. But I would not know how to generate such a background without first using the theory to gain knowledge of the signal through the "XANES" region of the EXAFS data. Also included are the Athena and Artemis project files used to generate the figures in this tutorial, so that you can follow along.

Thank you to Simon Bare of UOP LLC for donating the MoO3 data for this tutorial.

1. Open the moo3-tutorial.apj file in Athena. The first data set contains the MoO3 data, with all default values for background removal. Take a look at the default background, chi(k) data, and FT.

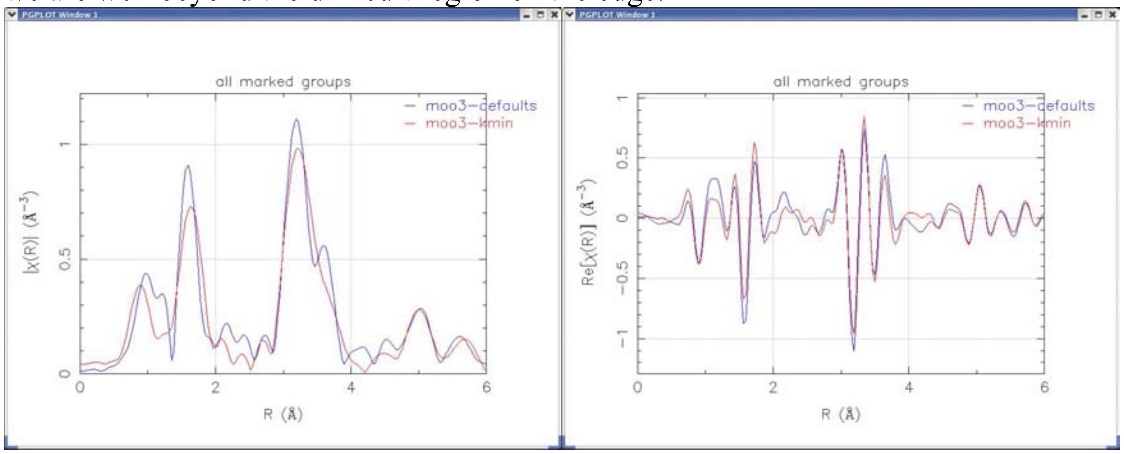






2. If the background through the XANES region is "good" there should be little change in the FT by including or excluding the low k-region of the chi(k) data.

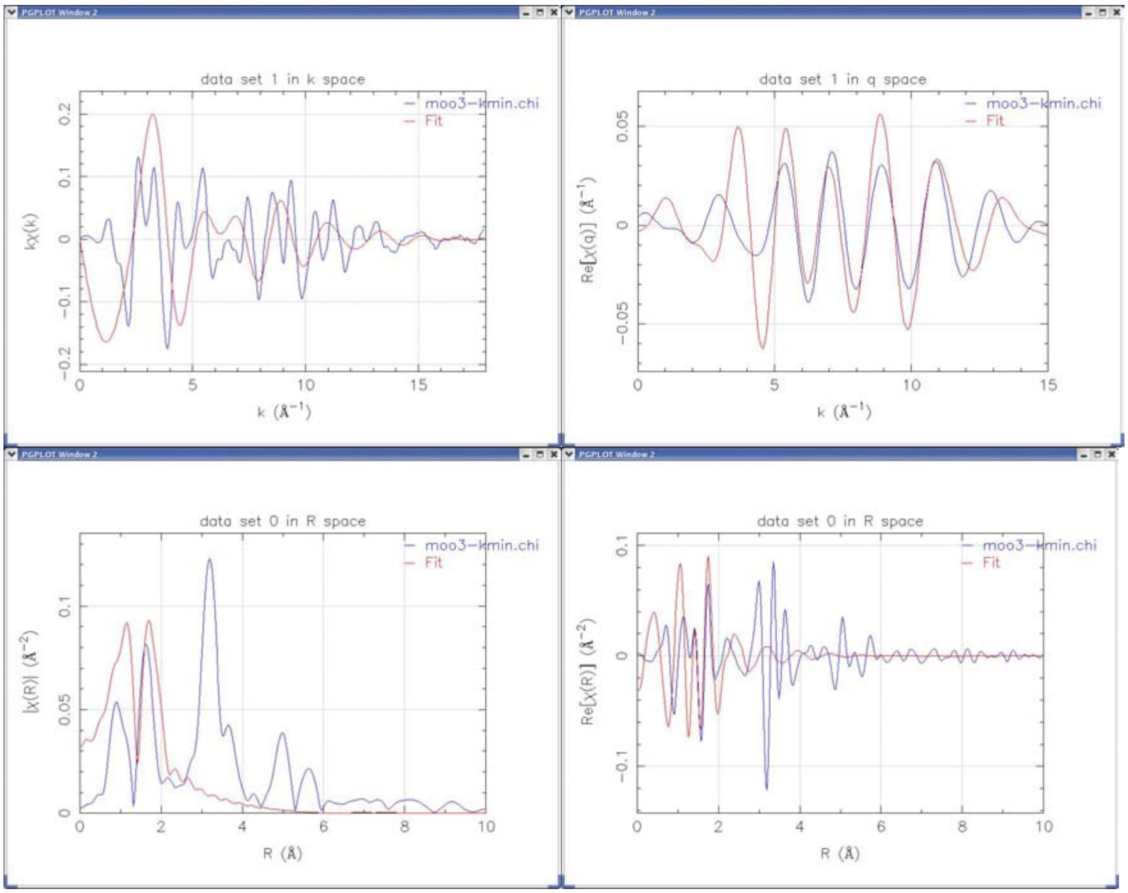
Make a copy of the original data set and call it moo3-kmin.
To test low k-region chi(k) data move kmin in the FT range from default 2 Å-1 to 4 Å-1. Look at the xmu(E) and chi(k) data above to see where 4 Å-1 is at on the edge. At 4 Å-1 we are well beyond the difficult region on the edge.



3. See the change in the FT of the data through the first peak region, so only use the data from 4 Å-1. Pull this data set into Athena.

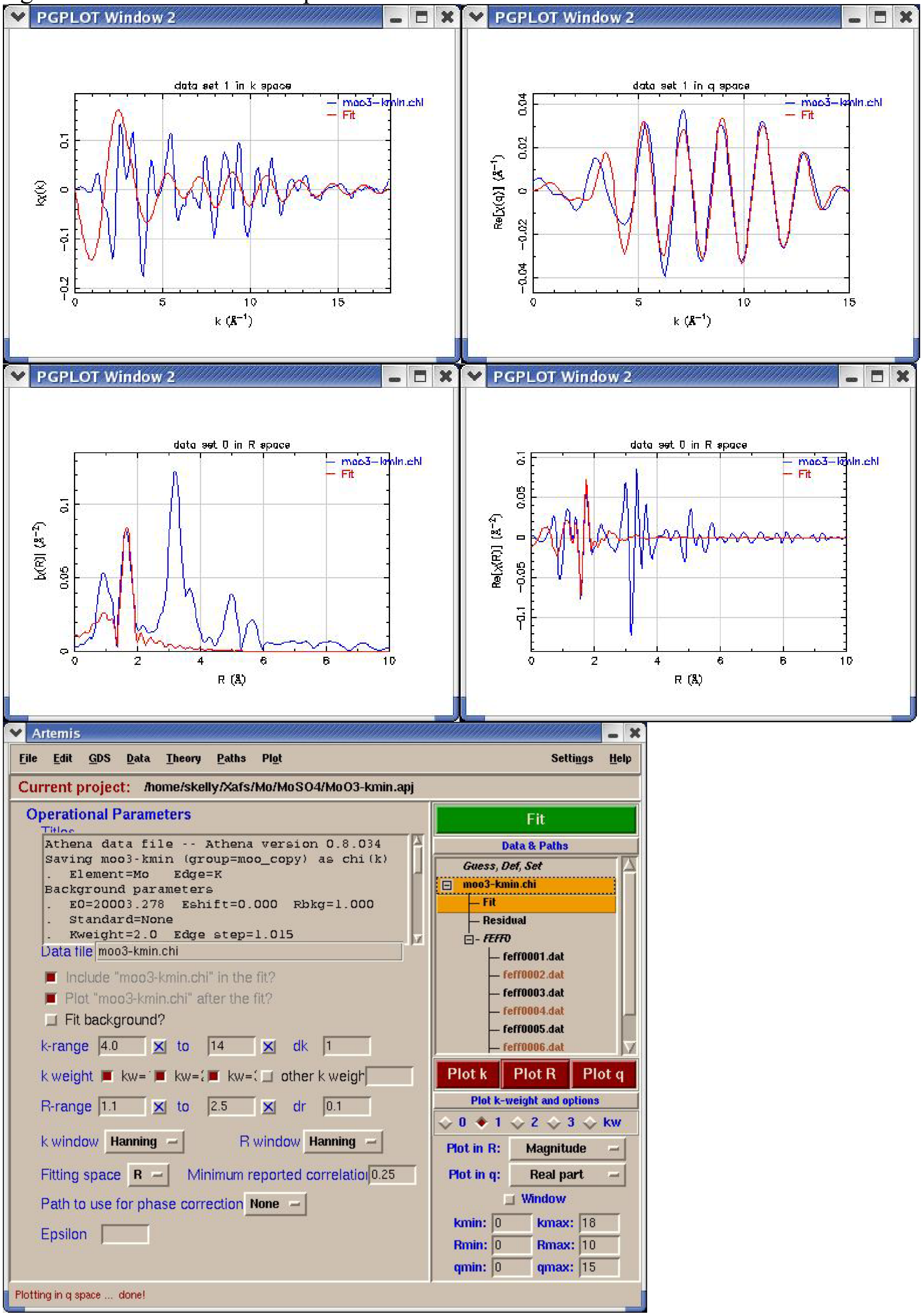
4. Open the Artemis project file Moo3-kmin.apj and compare the theory to the data.

Compare theory and data, using kmin = 4 Å-1 in the FT of the data.
Theory consists of three paths
2 Oxygen at 1.70 Å
2 Oxygen at 1.94 Å
2 Oxygen at 2.30 Å
For comparison set Ezero=0, sigma2=0.003, delr=0 for all paths.



This theory looks like it will work for this data set.
Q-data shows that the data and the theory are not aligned very well.
K-data and theory shows that the theory has the same overall shape.
FT of the data shows that the background needs to be fixed by the misfit at low R.

5. Fit the theory to the data, push the big green fit button. Set Ezero=0, determine sigma2 and delr for all three paths.

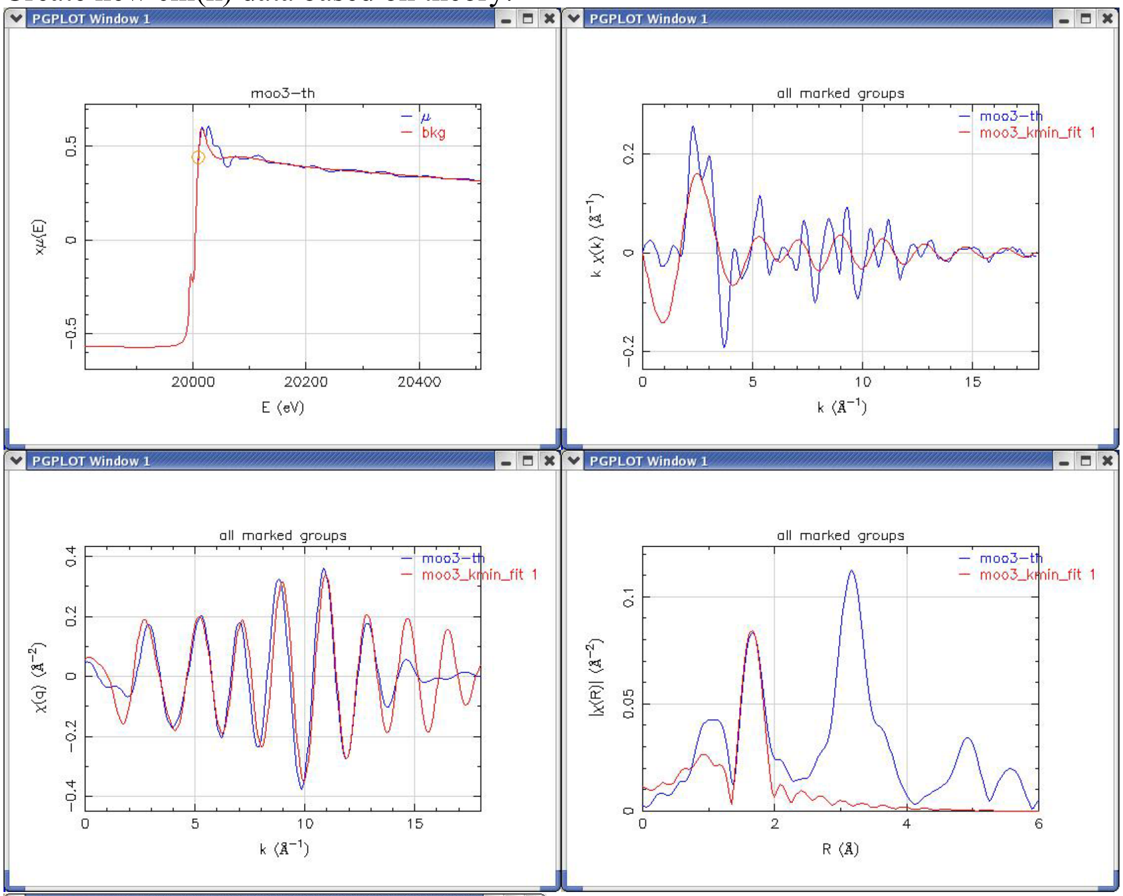


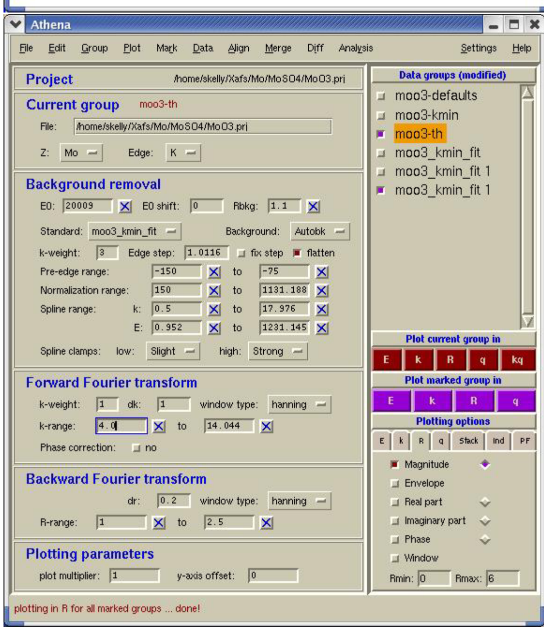
Save the chi(k) for the fit to disk to read it into Athena.

6. Produce a chi(k) theory that resembles the data.

The chi(k) fit is called moo3-kmin-fit use this data set as a standard for the moo3-th data set.

Create new chi(k) data based on theory:





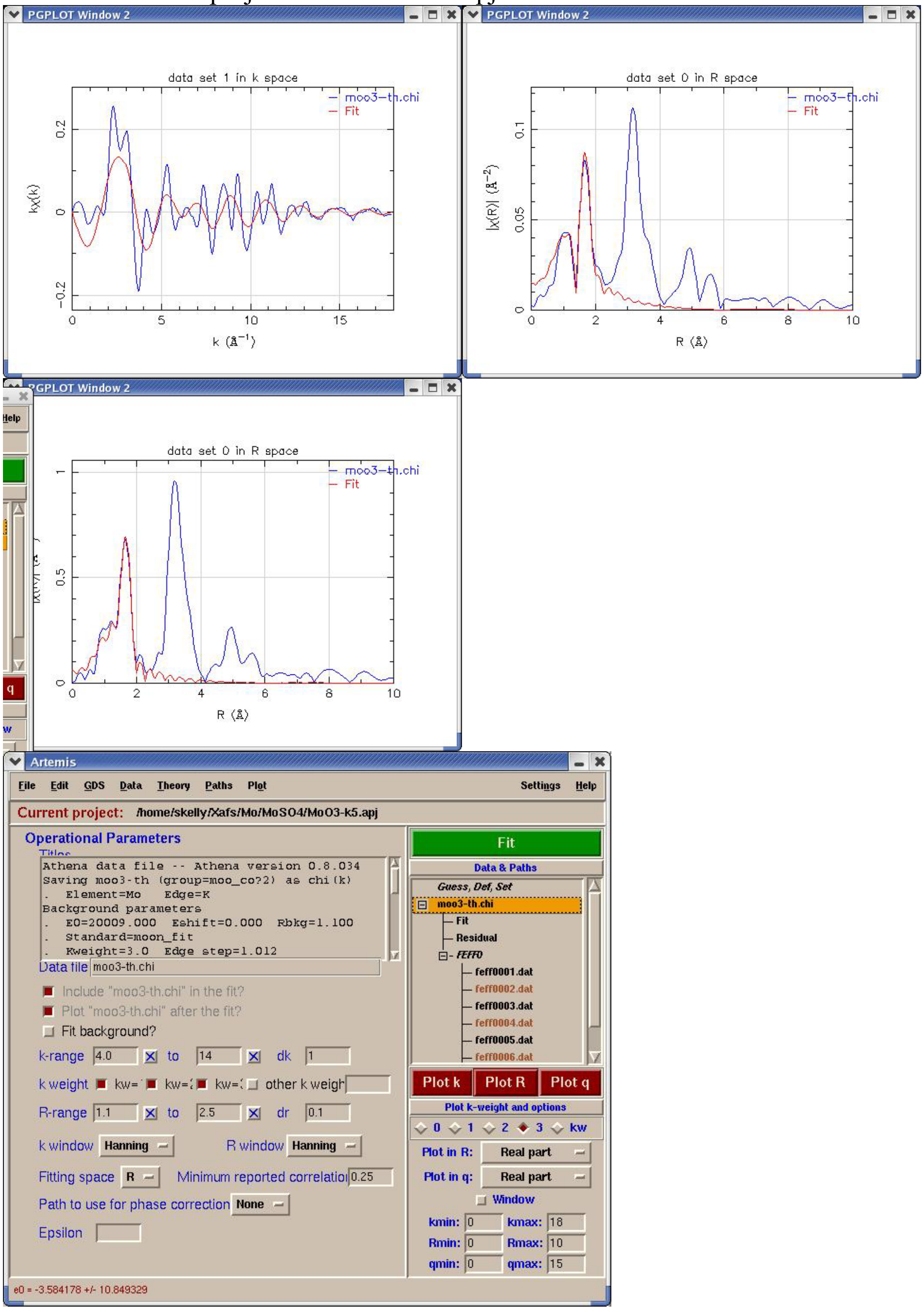
Things to notice:

- Xmu(E) data shows a “nice” shape through the edge region.
- Ezero is “on the edge”
- Chi(k) and chi(Q) data show that the data and theory are better aligned.
- FT of data and theory shows similar shape.

How we got here:

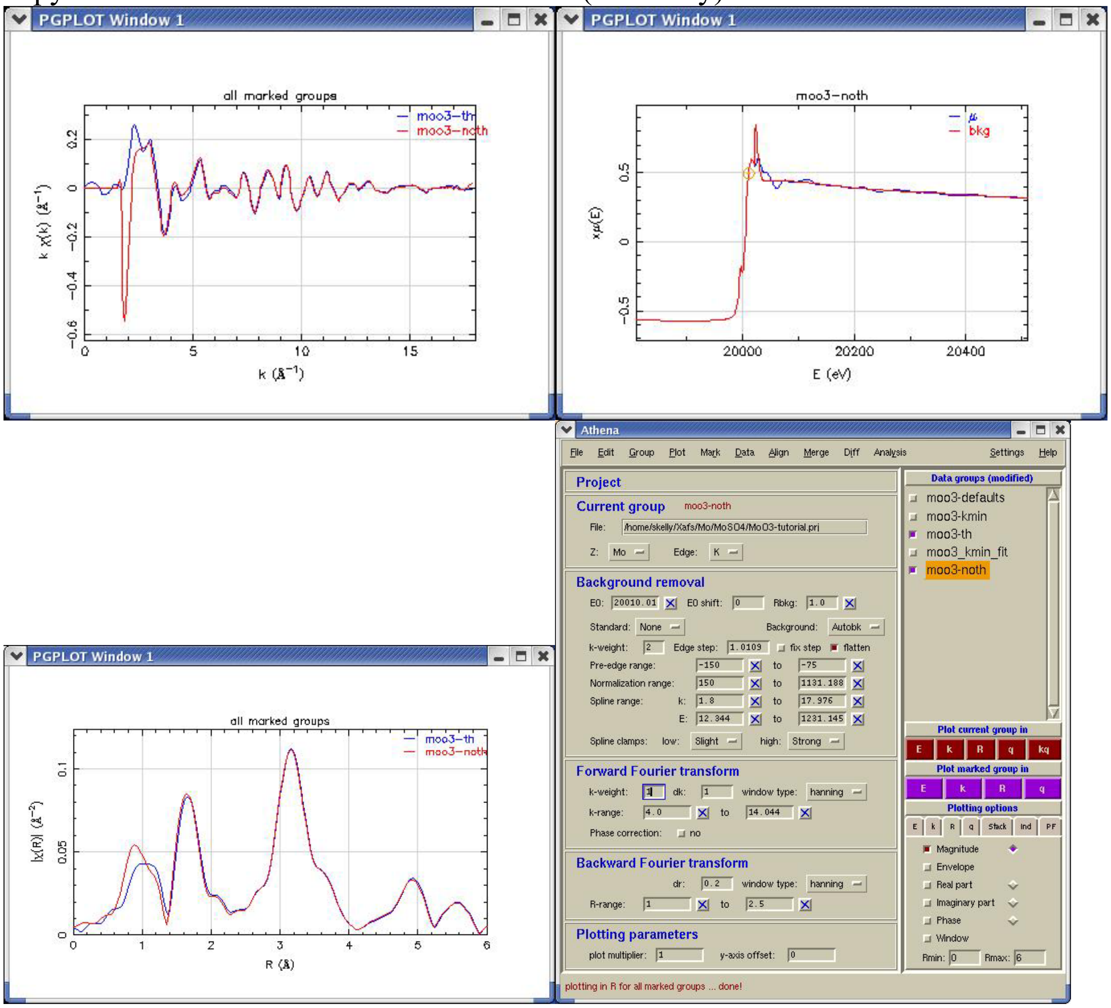
1. Move Ezero up by comparing the chi(k) data to the theory.
2. Increase rbkg from 1.0 to 1.1.
3. Increase the low spline clamp from none to slight.
4. Save the new chi(k) data to dist to read it into Artemis.

7. Fit the new chi(k) data. Save chi(k) data to disk and read it into Artemis. Open the artemis project file Moo3-final.apj.



Notice that the background and the theory follow each other nicely through the low R-range for all three k-weight used in the FT of the data.

Extra: See if we can reproduce the same chi(k) data without using a theory: Make a copy of the Moo3 data set called Moo3-noth (no theory).



This chi(k) data set moo3-noth uses no theory, and comes close to reproducing the same FT. I needed to increase kmin value and the background is not as "pretty"