

# Basics of EXAFS Data Processing

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**Honeywell**

- Introduction to Artemis
- Modeling Cu foil
- Background subtraction using theory
- Modeling U to determine neighboring atom type
- Multiple data set modeling

- M Newville. "IFEFFIT: interactive EXAFS analysis and FEFF fitting." J. Synch. Rad. **8**: pp 322-324, 2001. <http://cars9.uchicago.edu/ifeffit/>
- J J Rehr. "*Ab initio* multiple scattering X-ray absorption fine structure and X-ray absorption near edge structure code". University of Washington: pp, 1995. <http://leonardo.phys.washington.edu/feff/>
- E A Stern, M Newville, B Ravel, Y Yacoby and D Haskel. "The UWXAFS analysis package: Philosophy and details." Physica B **208 & 209**: pp 117-120, 1995.

# Artemis

Theory

Variables

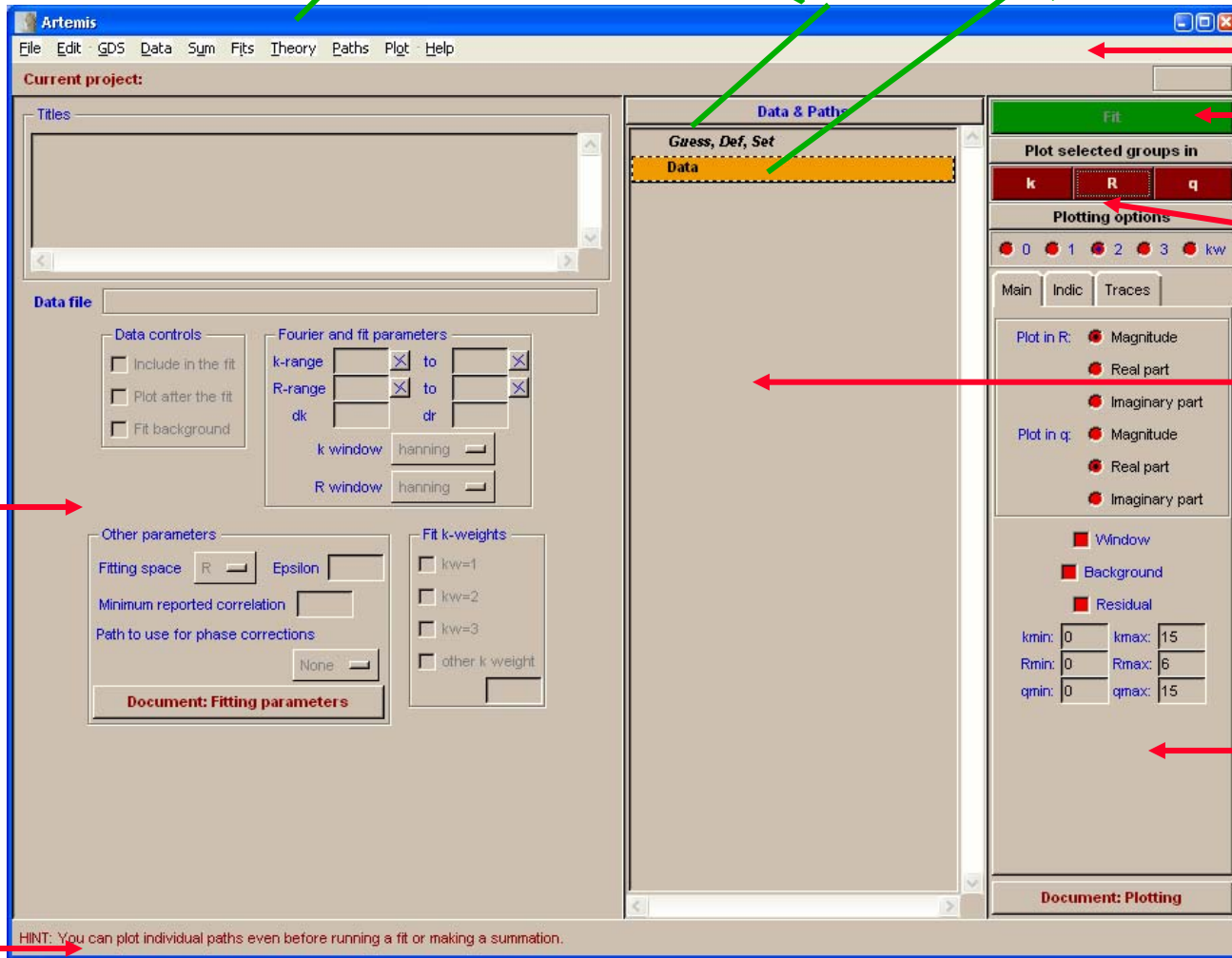
Data: input from Athena

Project Name:

Data display area:

Changes depending on selected information from Data and Paths list

Echo Area: Messages from Artemis



Menu:

Fit: optimize variables

Plot and Do buttons:

Data and Paths: Changes data display area

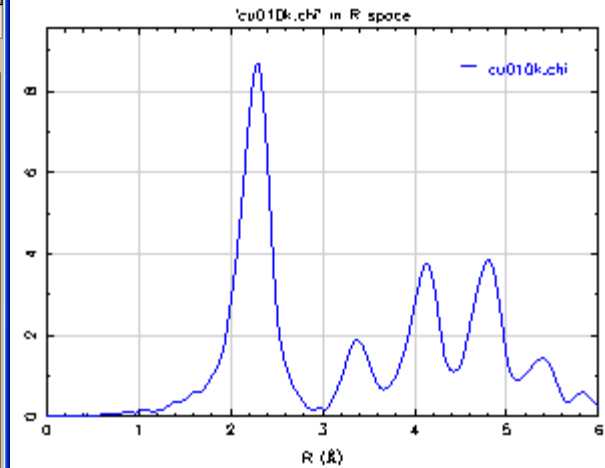
Plotting parameters

# Reading in $\chi$ Data

➤ File: open data file: F:\lfeffit\examples\Artemis\Cu\cu010k.chi

The screenshot shows the Artemis software interface with several panels:

- Titles:** Contains text from the data file: "Cu foil at 10K", "cu010k.dat : this file is part of the uwxafs 3.0", "data taken at NSLS beamline X-11A Sept 1992", "by M Newville, B Ravel, and Y Zhang", "foil of 99.999 Cu rolled and annealed to ~12 micr".
- Data file:** Shows the file name "cu010k.chi".
- Data controls:** Includes checkboxes for "Include in the fit", "Plot after the fit", and "Fit background".
- Fourier and fit parameters:** Includes fields for "k-range" (2 to 22.95), "R-range" (1 to 3), "dk" (1), and "dr" (0.0). It also has dropdown menus for "k window" and "R window", both set to "Hanning".
- Other parameters:** Includes "Fitting space" (R), "Epsilon" (0), "Minimum reported correlation" (0.25), and "Path to use for phase corrections" (None).
- Fit k-weights:** Includes checkboxes for "kw=1", "kw=2", "kw=3", and "other k weight".
- Fit panel:** Shows "Plot selected groups in" with buttons for "k", "R", and "q". The "R" button is selected. Below are "Plotting options" for "Plot in R:" and "Plot in q:" with radio buttons for "Magnitude", "Real part", and "Imaginary part". There are also checkboxes for "Window", "Background", and "Residual". At the bottom, there are input fields for "kmin", "kmax", "Rmin", "Rmax", "qmin", and "qmax".
- Data & Paths:** Shows the file "cu010k.chi" selected.
- Status bar:** Shows the message "Read data from C:\Program Files\lfeffit\examples\Artemis\Cu\cu010k.chi".



Data plotted in R-space

Title lines  
from data file

data file name

Fourier  
transform  
parameters

Message from Artemis

# Reading Data from Athena Project

➤ File: open data file: F:\lfeffit\examples\Athena\demos\align\_merge.prj

**list of data from Athena**

**Plot the data**

**Import the selected data set**

**Selected data set plotted**

Artemis

File Edit QDS Data Sum Fits Theory Paths Plot Help

Current project:

**Athena project** C:\Program Files\lfeffit\examples\Athena\demos\align\_merge.prj

Athena records

- Fe/Ga alloy scan 1
- Fe/Ga alloy scan 2
- Fe/Ga alloy scan 3

Header lines for Fe/Ga alloy scan 1

Guess, Def, Set

cu010k.chi

Plot as ...

- chi(k)
- |chi(R)|
- |chi(q)|
- Re[chi(R)]
- Re[chi(q)]
- Im[chi(R)]
- Im[chi(q)]

Use parameters from Athena project

Use default parameters

Import these data

Document: Importing Athena project data

Cancel and return to the main window

This is Athena record "Fe/Ga alloy scan 1" plotted in R-space

Fe/Ga alloy scan 1

Intensity (a.u.)

R (Å)

Plot in q:

- Magnitude
- Real part
- Imaginary part

Window

- Background
- Residual

kmin: 0 kmax: 15

Rmin: 0 Rmax: 6

qmin: 0 qmax: 15

Document: Plotting

# Atoms page

➤ File: open file: F:\lfeffit\examples\Artemis\Cu\atoms.inp

Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: modified

Atoms feff.inp Interpretation

Titles

Cu 222

Space group fcc

	Core	EI	X	Y	Z
A	1		0.00000	0.00000	0.00000
B					
C					
Alpha					
Beta					
Gamma					

Cluster size 7.00000

Edge K

Shift vector 0 0 0

Atom with a core hole

Data & Paths

Guess, Def, Set

cu010k.chi

FEFF0

Fit

Plot selected groups in

k R q

Plotting options

Plot in R: Magnitude Real part Imaginary part

Plot in q: Magnitude Real part Imaginary part

Window Background Residual

kmin: 0 kmax: 15

Rmin: 0 Rmax: 6

qmin: 0 qmax: 15

Run Atoms Document: Atoms

Message from Artemis

Importing crystallography file ... done!

# Theory input page (feff.inp)

➤ Click "Run Atoms"

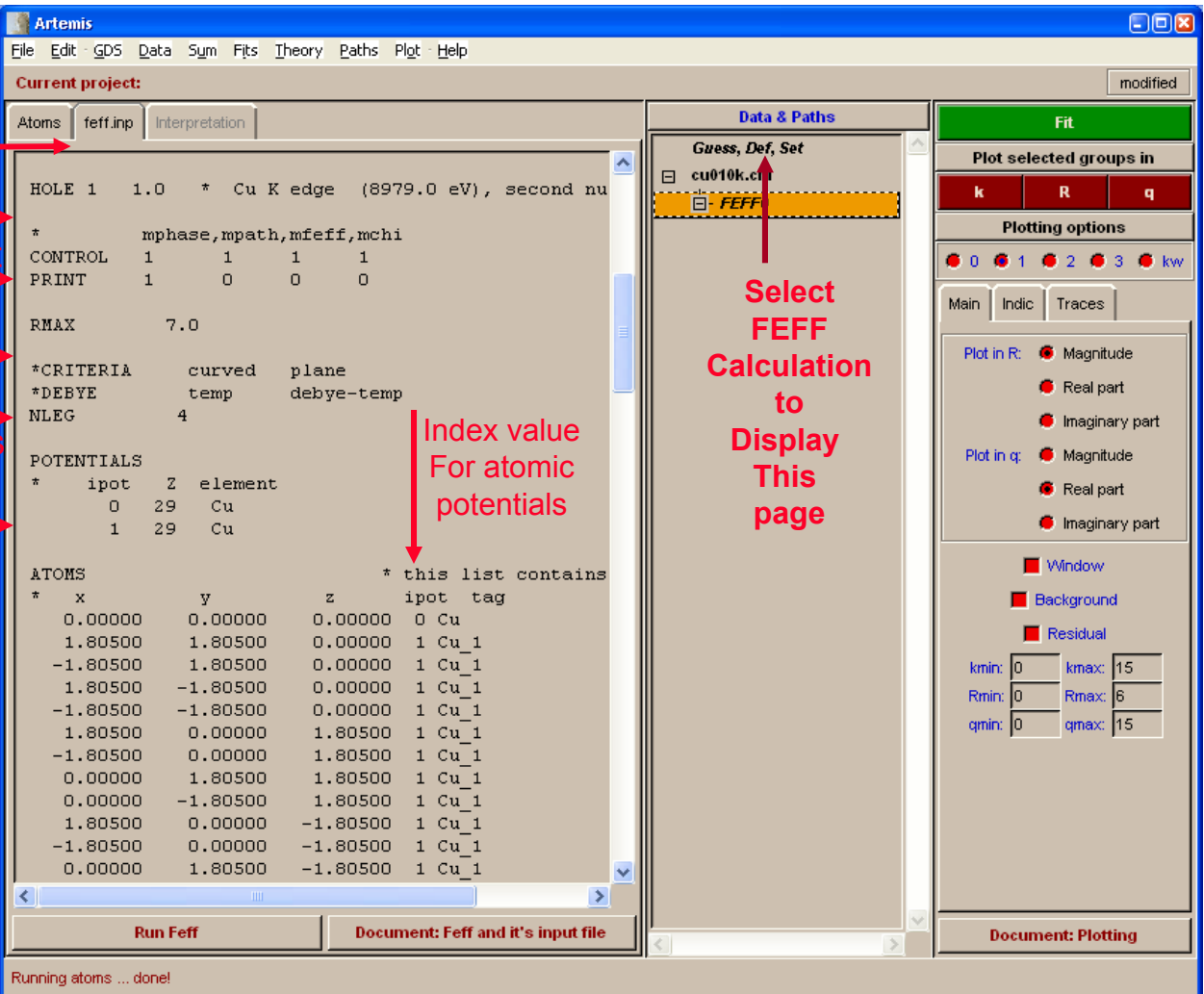
The screenshot shows the Artemis software interface with the following components and annotations:

- Feff.inp Tab:** A red arrow points to the 'feff.inp' tab in the 'Atom' section.
- Absorption lengths normalization correction:** A red arrow points to the text '\* total mu\*x=1: 4.06 microns, unit edge step' and another red arrow points to '\* Normalization correction: 0.00046 ang^2'.
- Crystallographic information From atoms.inp:** A red arrow points to the section starting with '\* The following crystallographic data were used:'.
- title lines hole number:** Red arrows point to 'TITLE Cu 222' and 'HOLE 1 1.0 \* Cu K edge (8979.0 eV), second nu'.
- Select FEFF Calculation to Display This page:** A red arrow points to the 'FEFF0' entry in the 'Data & Paths' panel.
- Run Feff:** A button at the bottom of the main window.
- Document: Feff and it's input file:** A label at the bottom of the main window.
- Document: Plotting:** A label at the bottom of the right-hand panel.

```
* This feff6 input file was generated by Artemis 0.
* Atoms written by and copyright (c) Bruce Ravel, 1
*
* --- * --- * --- * --- * --- * --- * --- * --- * --- * --- *
* total mu*x=1:      4.06 microns, unit edge step
* specific gravity = 8.971
*
* --- * --- * --- * --- * --- * --- * --- * --- * --- * --- *
* Normalization correction:  0.00046 ang^2
*
*
* +-----+
* The following crystallographic data were used:
*
* title      Cu 222
* space = F m -3 m
* a = 3.610 b = 3.610 c = 3.610
* alpha = 90.0 beta = 90.0 gamma = 90.
* core = Cu edge = K
* atoms
* ! elem  x      y      z      tag
* Cu 0.00000 0.00000 0.00000
*
* -----+
* TITLE Cu 222
*
* HOLE 1 1.0 * Cu K edge (8979.0 eV), second nu
*
* mphase,mpath,mfeff,mchi
* CONTROL 1 1 1 1
* PRINT 1 0 0 0
```

# Theory input page (feff.inp)

➤ Scroll feff.inp page downward



**Feff.inp Tab**

**Core Hole and S02 value**

**Toggle switches for different FEFF modules and output max path length**

**Control over the number of output paths**

**Atomic potential index list**

**List of atomic positions**

**Index value For atomic potentials**

**Select FEFF Calculation to Display This page**

**Run Feff**      **Document: Feff and it's input file**

**Document: Plotting**

```
HOLE 1 1.0 * Cu K edge (8979.0 eV), second nu
*
* mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0
RMAX 7.0
*CRITERIA curved plane
*DEBYE temp debye-temp
NLEG 4
POTENTIALS
* ipot Z element
0 29 Cu
1 29 Cu
ATOMS * this list contains
* x y z ipot tag
0.00000 0.00000 0.00000 0 Cu
1.80500 1.80500 0.00000 1 Cu_1
-1.80500 1.80500 0.00000 1 Cu_1
1.80500 -1.80500 0.00000 1 Cu_1
-1.80500 -1.80500 0.00000 1 Cu_1
1.80500 0.00000 1.80500 1 Cu_1
-1.80500 0.00000 1.80500 1 Cu_1
0.00000 1.80500 1.80500 1 Cu_1
0.00000 -1.80500 1.80500 1 Cu_1
1.80500 0.00000 -1.80500 1 Cu_1
-1.80500 0.00000 -1.80500 1 Cu_1
0.00000 1.80500 -1.80500 1 Cu_1
```



# Theory input page (feff.inp)

➤ Scroll feff.inp page downward and to the right

Check that the atomic  
Distances from the absorbing atom  
Are reasonable

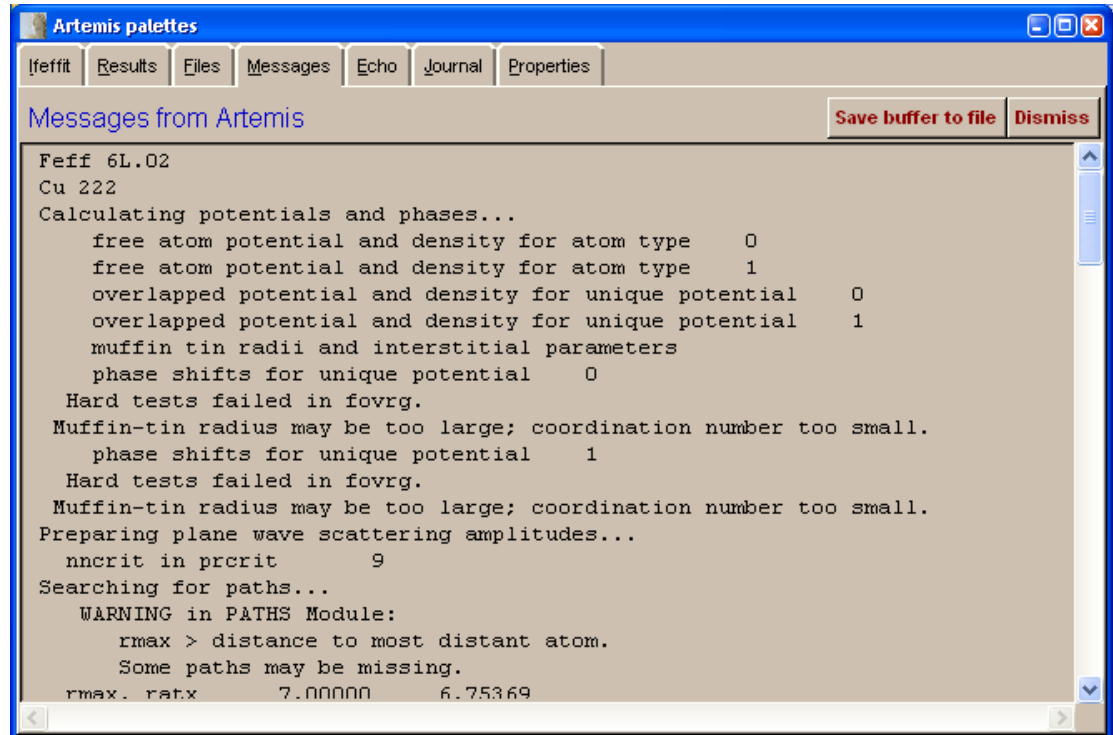
The screenshot shows the Artemis software interface. The main window displays the 'feff.inp' input file content, which is a list of atomic coordinates and distances. A red oval highlights the 'distance' column, and a red arrow points from the text 'Check that the atomic Distances from the absorbing atom Are reasonable' to this column. The 'Data & Paths' panel on the right shows the 'Guess, Def, Set' section with 'FEFF0' selected. A red arrow points from the text 'Select FEFF Calculation to Display This page' to the 'FEFF0' entry. The 'Fit' panel on the far right shows plotting options for 'k', 'R', and 'q'.

y	z	ipot	tag	distance
0.00000	0.00000	0	Cu	0.00000
1.80500	0.00000	1	Cu_1	2.55266
1.80500	0.00000	1	Cu_1	2.55266
-1.80500	0.00000	1	Cu_1	2.55266
-1.80500	0.00000	1	Cu_1	2.55266
0.00000	1.80500	1	Cu_1	2.55266
1.80500	1.80500	1	Cu_1	2.55266
-1.80500	1.80500	1	Cu_1	2.55266
0.00000	-1.80500	1	Cu_1	2.55266
0.00000	-1.80500	1	Cu_1	2.55266
1.80500	-1.80500	1	Cu_1	2.55266
-1.80500	-1.80500	1	Cu_1	2.55266
0.00000	0.00000	1	Cu_2	3.61000
0.00000	0.00000	1	Cu_2	3.61000
3.61000	0.00000	1	Cu_2	3.61000
-3.61000	0.00000	1	Cu_2	3.61000
0.00000	3.61000	1	Cu_2	3.61000
0.00000	-3.61000	1	Cu_2	3.61000
1.80500	1.80500	1	Cu_3	4.42133
1.80500	1.80500	1	Cu_3	4.42133
3.61000	1.80500	1	Cu_3	4.42133
3.61000	1.80500	1	Cu_3	4.42133
-1.80500	1.80500	1	Cu_3	4.42133
-1.80500	1.80500	1	Cu_3	4.42133
-3.61000	1.80500	1	Cu_3	4.42133
-3.61000	1.80500	1	Cu_3	4.42133
1.80500	3.61000	1	Cu_3	4.42133
1.80500	3.61000	1	Cu_3	4.42133

## Text messages during Feff calculation

- **Artemis Palettes**

- **lfeffit:** Shows the interface from Artemis to lfeffit. Artemis is just a nice interface to lfeffit. lfeffit does the work!
- **Results:** Shows the results page from a fit of the theory to the data.
- **Files:** Shows data files.
- **Messages:** Shows output from Feff.
- **Echo:** Shows entire message from Artemis Echo area
- **Journal:** Useful place to make notes.
- **Properties:** Notes about the current project file.



```
Artemis palettes
lfeffit Results Files Messages Echo Journal Properties
Messages from Artemis Save buffer to file Dismiss
Feff 6L.02
Cu 222
Calculating potentials and phases...
  free atom potential and density for atom type    0
  free atom potential and density for atom type    1
  overlapped potential and density for unique potential    0
  overlapped potential and density for unique potential    1
  muffin tin radii and interstitial parameters
  phase shifts for unique potential    0
Hard tests failed in fovrg.
Muffin-tin radius may be too large; coordination number too small.
  phase shifts for unique potential    1
Hard tests failed in fovrg.
Muffin-tin radius may be too large; coordination number too small.
Preparing plane wave scattering amplitudes...
nncrit in prcrit    9
Searching for paths...
WARNING in PATHS Module:
  rmax > distance to most distant atom.
  Some paths may be missing.
rmax. ratx    7.00000    6.75369
```

# Feff paths: feffxxx.dat

- **Degen:** Degeneracy of the path (number of identical scattering paths)

- **reff:** Initial half path length (bond length for single scattering path)

- **amp:** Estimate of amplitude of path relative to first path.

- **fs:** Number of forward scattering events.

- **scattering path:** atoms scattering photoelectron, [+] symbol represents core atom.

Artemis

File Edit GD5 Data Sum Fits Theory Paths Plot Help

Current project: modified

Atoms feff.inp Interpretation

Interpretation of the FEFF Calculation

# TITLE Cu 222  
# Central atom: Copper (29) K edge energy = 8979 eV  
# The central atom is denoted by this token: [+]  
# Cluster size = 7.0 Angstroms, containing 135 atoms.  
# Curved wave criteria = 2.5.

#	Degen	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00	[+]	Cu_1 [+]
2	6	3.610	22.98	[+]	Cu_2 [+]
3	48	3.829	10.59	[+]	Cu_1 Cu_1 [+]
4	48	4.358	8.65	[+]	Cu_2 Cu_1 [+]
5	24	4.421	55.40	[+]	Cu_3 [+]
6	48	4.763	10.62	[+]	Cu_1 Cu_1 [+]
7	96	4.763	21.84	[+]	Cu_3 Cu_1 [+]
8	12	5.105	18.93	[+]	Cu_4 [+]
9	12	5.105	8.46	[+]	Cu_1 Cu_1 [+]
10	24	5.105	43.72	1	[+] Cu_4 Cu_1 [+]
11	12	5.105	8.20	1	[+] Cu_1 [+] Cu_1 [+]
12	12	5.105	3.56	[+]	Cu_1 [+] Cu_1 [+]
14	12	5.105	32.79	2	[+] Cu_1 Cu_4 Cu_1 [+]
15	48	5.105	3.26	[+]	Cu_1 Cu_1 Cu_1 [+]
18	48	5.292	4.14	[+]	Cu_3 Cu_1 [+]
19	48	5.292	4.09	[+]	Cu_3 Cu_2 [+]
20	96	5.698	2.73	[+]	Cu_3 Cu_1 [+]
21	48	5.698	4.80	[+]	Cu_3 Cu_3 [+]

Document: Feff interpretation

All done running FEFF.

Data & Paths

Guess, Def, Set

cu010k.chi

FEFF0

- Path 1: [Cu\_1]
- Path 2: [Cu\_2]
- Path 3: [Cu\_1 Cu\_1]
- Path 4: [Cu\_2 Cu\_1]
- Path 5: [Cu\_3]
- Path 6: [Cu\_1 Cu\_1]
- Path 7: [Cu\_3 Cu\_1]
- Path 8: [Cu\_4]
- Path 9: [Cu\_1 Cu\_1]
- Path 10: [Cu\_4 Cu\_1]

Fit

Plot selected groups in

k R q

Plotting options

0 1 2 3 kw

Main Indic Traces

Plot in R:  Magnitude  Real part  Imaginary part

Plot in q:  Magnitude  Real part  Imaginary part

Window  Background  Residual

kmin: 0 kmax: 15  
Rmin: 0 Rmax: 6  
qmin: 0 qmax: 15

Document: Plotting

S I Zabinsky, J J Rehr, A Ankudinov, R C Albers and M J Eller. "Multiple-scattering calculations of X-ray-absorption spectra." *Phys. Rev. B* **52**(4): pp 2995-3009, 1995.

# Path Description

➤ Click on Path1 in the Data & Paths list

Feff calculation

Path description

parameters

The screenshot shows the Artemis software interface with the following components:

- Current project:** FEFF0: Path 1: [Cu\_1]
- FEFF0: Path 1: [Cu\_1] settings:**
  - Plot after the fit
  - Include in the fit
  - Make this path the default after the fit
- Path description:**

[+] Cu\_1 [+]

2 legs Reff=2.5527 amp=100.000 degen=12

leg 1: 0.00000 1.80500 -1.80500 1 Cu  
rleg=2.5527 beta=180.000

leg 2: 0.00000 0.00000 0.00000 0 Cu  
rleg=2.5527 beta=180.000
- Path parameter math expressions:**

label:	
N:	12 X S02: amp
delE0:	enot
delR:	delr
sigma^2:	ss
Ei:	
3rd:	
4th:	
- Data & Paths list:**
  - cu010k.chi
  - FEFF0
    - Path 1: [Cu\_1] (highlighted)
    - Path 2: [Cu\_2]
    - Path 3: [Cu\_1 Cu\_1]
    - Path 4: [Cu\_2 Cu\_1]
    - Path 5: [Cu\_3]
    - Path 6: [Cu\_1 Cu\_1]
    - Path 7: [Cu\_3 Cu\_1]
    - Path 8: [Cu\_4]
    - Path 9: [Cu\_1 Cu\_1]
    - Path 10: [Cu\_4 Cu\_1]
- Fit panel:**
  - Plot selected groups in: k, R, q (R is selected)
  - Plotting options: 0, 1, 2, 3, kw
  - Plot in R: Magnitude, Real part, Imaginary part
  - Plot in q: Magnitude, Real part, Imaginary part
  - Window, Background, Residual checkboxes
  - Scale ranges: kmin: 0, kmax: 15; Rmin: 0, Rmax: 6; qmin: 0, qmax: 15
- Status bar:** All done running FEFF.

# The EXAFS Equation

- E. A. Stern and S M Heald Basic principles and applications of EXAFS. *Handbook of Synchrotron Radiation*. E. E. Koch. New York, North-Holland. **10**: pp 995-1014, 1983.
- E. A. Stern. "Theory of the extended x-ray-absorption fine structure." *Phys Rev B* **10**(8): pp 3027-3037, Oct 1974.
- E A Stern. "Structural determination by X-ray Absorption." *Contemp. Phys* **19**(4): pp 239-310, 1978.

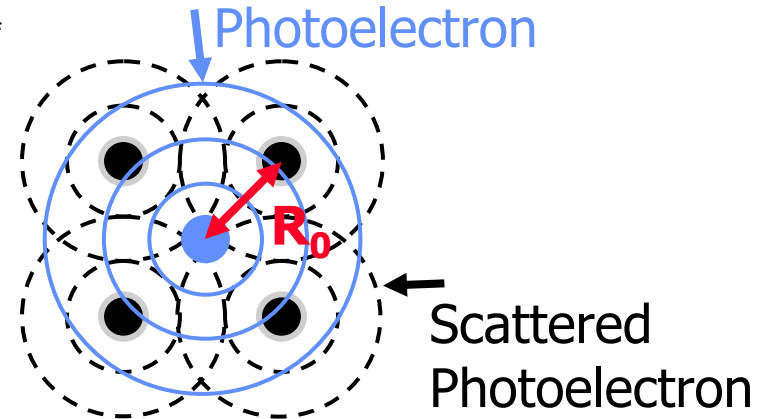
$$\chi(k) = \sum_i \chi_i(k)$$

with each path written as:

$$\chi_i(k) = \left( \frac{N_i S_0^2 F_i(k)}{k R_i^2} \sin(2kR_i + \phi_i(k)) \exp(-2\sigma_i^2 k^2) \exp(-2R_i/\lambda(k)) \right)$$

$$R_i = R_0 + \Delta R$$

$$k^2 = 2 m_e (E - E_0) / \hbar$$



$F_i(k)$  effective scattering amplitude  
 $\phi_i(k)$  effective scattering phase shift  
 $\lambda(k)$  mean free path  
 $R_0$  initial path length

$N_i$  degeneracy of path  
 $S_0^2$  passive electron reduction factor  
 $E_0$  energy shift  
 $\Delta R$  change in half-path length  
 $\sigma_i^2$  mean squared displacement

Feff calculates the theoretical scattering amplitude  $F(k)$  effective, hence the name Feff.

# Path Parameters

- To produce a theoretical model each path must have a value for each of these parameters.
- Artemis makes a guess for these expressions.
- These values can originate from numbers or math expressions.

**S02** passive electron reduction factor

**N** degeneracy of path

**E0** energy shift

**delR** change in half-path length

**sigma^2** mean squared displacement of the half path length

The screenshot shows the Artemis software interface. The main window is titled "Artemis" and has a menu bar with "File", "Edit", "GD5", "Data", "Sum", "Fits", "Theory", "Paths", "Plot", and "Help". The "Current project" is "FEFF0: Path 1: [Cu\_1]". The "Data & Paths" panel shows a list of paths: Path 1: [Cu\_1], Path 2: [Cu\_2], Path 3: [Cu\_1 Cu\_1], Path 4: [Cu\_2 Cu\_1], Path 5: [Cu\_3], Path 6: [Cu\_1 Cu\_1], Path 7: [Cu\_3 Cu\_1], Path 8: [Cu\_4], Path 9: [Cu\_1 Cu\_1], and Path 10: [Cu\_4 Cu\_1]. The "Path parameter math expressions" panel shows a table with columns for "label", "N", "delE0", "delR", "sigma^2", "Ei", "3rd", and "4th". The "Path parameter math expressions" panel is highlighted with a red arrow pointing to the "S02" parameter. The "Fit" panel shows "Plot selected groups in" with buttons for "k", "R", and "q". The "Plotting options" panel shows "Plot in R:" with radio buttons for "Magnitude", "Real part", and "Imaginary part", and "Plot in q:" with radio buttons for "Magnitude", "Real part", and "Imaginary part". The "Window" panel shows "Background" and "Residual" checkboxes. The "kmin", "kmax", "Rmin", "Rmax", "qmin", and "qmax" fields are set to 0 and 15. The "Document: Paths and path parameters" and "Document: Plotting" panels are visible at the bottom. The status bar at the bottom says "All done running FEFF0."

➤ Click "Guess, Def, Set" in the Data & Paths list

# EXAFS parameters

- **Guess:** Optimize parameter in fit.
- **Def:** Define a parameter to a given value but re-evaluate it during the fit
- **Set:** Set a value to a given value. Determine value once.
- **Skip:** Do not use this parameter.
- **Restrain:** penalty that can be added to the fit.

- **Define:** Define parameter to value given.
- **New:** Make a new parameter.
- **Grab:** Set the value to the best-fit value from the fit.
- **Discard:** remove parameter.
- **Hide:** Hide editing area

The screenshot shows the Artemis software interface. The main window is titled 'Artemis' and has a menu bar with 'File', 'Edit', 'GDS', 'Data', 'Sum', 'Fits', 'Theory', 'Paths', 'Plot', and 'Help'. Below the menu bar is a 'Current project:' section. The main area is divided into several panels:

- Parameters Table:** A table with columns '#', 'Name', and 'Math Expression'. It contains four rows:

#	Name	Math Expression
1	d: amp	1
2	s: enot	0
3	g: delr	0
4	g: ss	0.003
- Data & Paths:** A tree view showing the data file 'cu010k.chi' and its paths: Path 1: [Cu\_1], Path 2: [Cu\_2], Path 3: [Cu\_1 Cu\_1], Path 4: [Cu\_2 Cu\_1], Path 5: [Cu\_3], Path 6: [Cu\_1 Cu\_1], Path 7: [Cu\_3 Cu\_1], Path 8: [Cu\_4], Path 9: [Cu\_1 Cu\_1], Path 10: [Cu\_4 Cu\_1].
- Fit Panel:** A panel on the right with a green 'Fit' button. It contains a table for 'Plot selected groups in' with columns 'k', 'R', and 'q'. Below it are 'Plotting options' for 'Plot in R' and 'Plot in q', each with radio buttons for 'Magnitude', 'Real part', and 'Imaginary part'. There are also checkboxes for 'Window', 'Background', and 'Residual', and input fields for 'kmin', 'kmax', 'Rmin', 'Rmax', 'qmin', and 'qmax'.
- Edit selected parameter:** A dialog box at the bottom showing the parameter 'ss' with a value of '0.003'. It has radio buttons for 'Guess', 'Def', 'Set', 'Skip', 'Restrain', and 'After'. Below these are buttons for 'Undo edit', 'New', 'Grab', 'Discard', and 'Hide'.

Red arrows point from the text descriptions to the corresponding elements in the software interface. A large red text box in the center of the interface reads: 'Name of parameters that YOU have created to define the required values for each path'.

➤ Click "Fit" to optimize these values

# Fit Results

Artemis palettes

Results from the last fit

Raw log file Save Dismiss

Project title : Fitting cu010k.chi  
Comment : Fit #1  
Prepared by :  
Contact :  
Started : 12:38:31 on 26 June, 2009  
This fit at : 14:41:50 on 27 June, 2009  
Environment : Artemis 0.8.013 using Windows XP, perl 5.008008, Tk 804.027, a  
Data sets : "cu010k.chi"  
Fit label : fit 1  
Figure of merit : 1

=====  
Independent points = 21.187500000  
Number of variables = 4.000000000  
Chi-square = 1078.130989819  
Reduced Chi-square = 62.727621226  
R-factor = 0.010391311  
Measurement uncertainty (k) = 0.000914479  
Measurement uncertainty (R) = 0.003911955  
Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):  
amp = 0.8626890 +/- 0.0435050 (1.0000)  
enot = 4.8357170 +/- 0.4306520 (0.0000)  
ss = 0.0031660 +/- 0.0003500 (0.0030)  
alpha = -0.0030710 +/- 0.0010070 (0.0000)

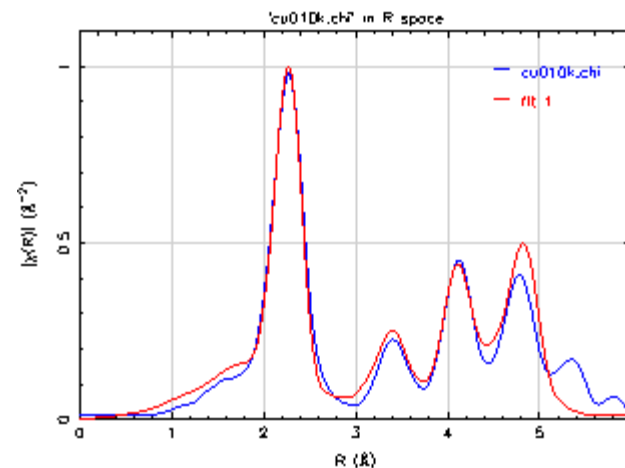
Correlations between variables:  
enot and alpha --> 0.8711  
All other correlations are below 0.25

Best fit values with uncertainties

Initial guessed value

Statistical quality of Fit

Your parameters





# Fit Results

```
==== Paths used to fit cu010k.chi

FEFFO: Path 1: [Cu 1] ..
feff = D:\Documents and Settings\E446095\Application Data\horae\stash\artem:
id = reff= 2.5527, nlegs= 2, path= Cu<->Cu
label =
r = 2.544859
degen = 12.000000
s02 = 0.862689
e0 = 4.835717
dr = -0.007841
ss2 = 0.003166
3rd = 0.000000
4th = 0.000000
ei = 0.000000

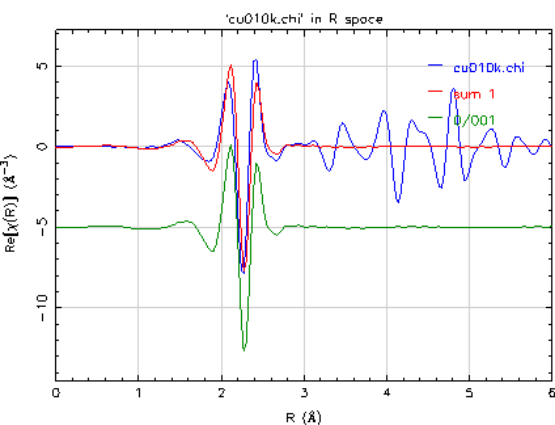
FEFFO: Path 2: [Cu 2] ..
feff = D:\Documents and Settings\E446095\Application Data\horae\stash\artem:
id = reff= 3.6100, nlegs= 2, path= Cu<->Cu
label =
r = 3.598912
degen = 6.000000
s02 = 0.862689
e0 = 4.835717
dr = -0.011088
ss2 = 0.003166
3rd = 0.000000
4th = 0.000000
ei = 0.000000

FEFFO: Path 3: [Cu 1 Cu 1] ..
feff = D:\Documents and Settings\E446095\Application Data\horae\stash\artem:
id = reff= 3.8290, nlegs= 3, path= Cu->Cu->Cu->Cu
```

The value used for each EXAFS parameter for each path included in the fit.

Used as a diagnostic tool when models do not work as expected

# Example: Cu foil



## GSD Info

Artemis

File Edit GDS Data Sum Fits Theory Pal

Current project: C:/Program Files/lfeffit/examp

#	Name	Math Expression
1	g: amp	0.9
2	g: enot	0
3	g: delr	0
4	g: sigsqr	0.003
5	d: signor	0.00052

## Path Info

Plot after the fit  Include in the fit

Make this path the default after the fit

[+] Cu\_1 [+]

2 legs Reff=2.5527 amp=100.000 degen=12

leg 1: 0.00000 1.80500 -1.80500 1 Cu  
rleg=2.5527 beta=180.000

leg 2: 0.00000 0.00000 0.00000 0 Cu  
rleg=2.5527 beta=180.000

Path parameter math expressions

label:

N: 12 X S02 amp

delE0: enot

delR: delr

sigma^2: sigsqr + signor

Ei:

3rd:

4th:

Guess, Def, Set

cu010k.chi

- Sum
- sum 1
  - FEFF0
    - feff0001.dat
    - feff0002.dat
    - feff0003.dat
    - feff0004.dat
    - feff0005.dat

## Data Parameters

Data file: cu010k.chi

Data controls

- Include data in the fit?
- Plot data after the fit?
- Fit background

Fourier and fit parameters

k-range: 2.5 to 18

R-range: 1.396 to 2.793

dk: 1 dr: 0.5

k window: Hanning

R window: Hanning

Other parameters

Fitting space: R Epsilon: 0

Minimum reported correlation: 0.25

Path to use for phase corrections: None

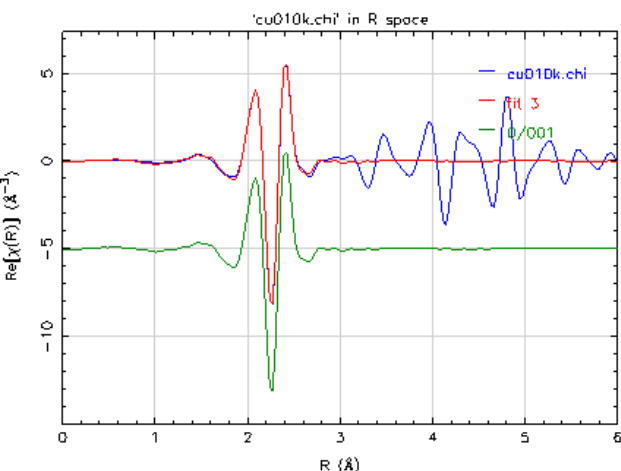
Fit k-weights

- kw=1
- kw=2
- kw=3
- other k weight

Document: Fitting parameters

- Example from c:\Program Files\lfeffit\examples\Artemis
- Set up variables for first shell and give them reasonable values
- Sum paths to see how the theory corresponds to the data
- Notice strong signal due to 1<sup>st</sup> Cu neighbor is in about the right place for the data. Overall shape is similar
- Make sure that fit range is appropriate and choose kw for fit

# Cu First Shell Model Results



## GSD Info

#	Name	Math Expression
1	g: amp	0.908747 (0.020905)
2	g: enot	5.487727 (0.267428)
3	g: delr	-0.004584 (0.001284)
4	g: sigsqr	0.002945 (0.000132)
5	d: signor	0.00052

## Results Info

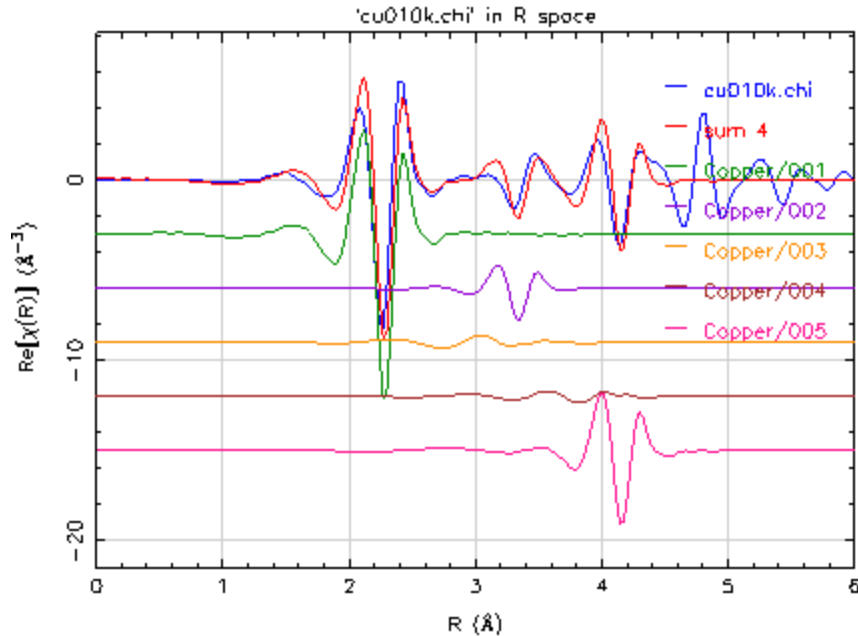
```
Independent points      =      13.579101562
Number of variables    =      4.000000000
Chi-square             =     259.769677739
Reduced Chi-square     =     27.118375982
R-factor               =      0.001326741
Measurement uncertainty (k) = 0.001130698
Measurement uncertainty (R) = 0.004441269
Number of data sets    =      1.000000000
```

```
Guess parameters +/- uncertainties (initial guess):
amp      =      0.9087470 +/-      0.0209050
enot     =      5.4877270 +/-      0.2674280
delr     =     -0.0045840 +/-      0.0012840
sigsqr   =      0.0029450 +/-      0.0001320

Def parameters (using "FEFFO: feff0001.dat"):
signor   =      0.0005200
```

- Data and Model are in good agreement
- GSD values are reasonable

# Cu: Three Shell Model



### Path Info

Make this path the default after the fit

[+] Cu\_1 [+]

2 legs Reff=2.5527 amp=100.000 degen=12

leg 1:	0.00000	1.80500	-1.80500	1	Cu
	rleg=2.5527	beta=180.000			
leg 2:	0.00000	0.00000	0.00000	0	Cu
	rleg=2.5527	beta=180.000			

Path parameter math expressions

label:	
N:	12 <input checked="" type="checkbox"/> S02: amp
delE0:	enot
delR:	alpha*reff
sigma^2:	debye(temp, theta) + signor
Ei:	
3rd:	
4th:	

cu010k.chi  
Copper

- feff0001.dat
- feff0002.dat
- feff0003.dat
- feff0004.dat
- feff0005.dat
- feff0006.dat
- feff0007.dat
- feff0008.dat
- feff0009.dat
- feff0010.dat
- feff0011.dat
- feff0012.dat
- feff0014.dat
- feff0015.dat

## GSD Info

Artemis

File Edit GDS Data Sum Fits Theory

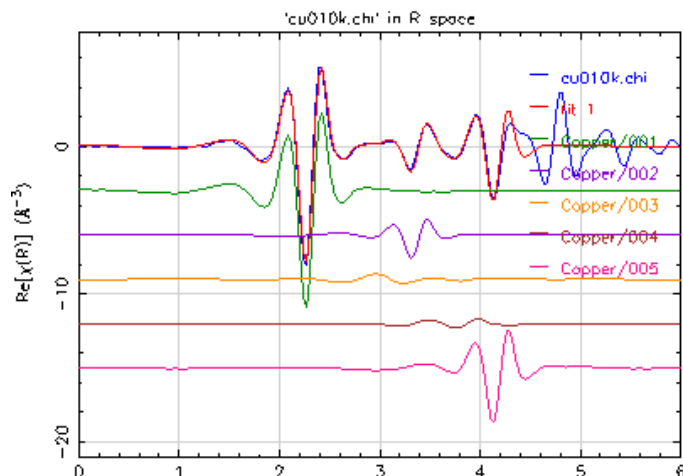
Current project: C:/Program Files/feffit/e

#	Name	Math Expression
1	g: amp	1
2	g: enot	0
3	g: alpha	0
4	s: temp	10
5	g: theta	350
6	s: signor	0.00052

- Use alpha to define path lengths
- Use Debye temperature to define  $\sigma^2$  values
- Each Single scattering path fits into a specific signal in the data

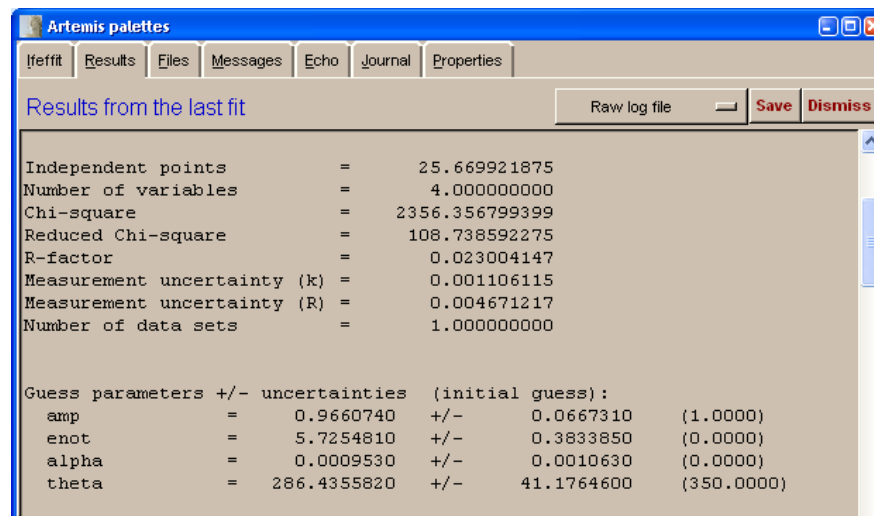
# Fitting results for three shell fit to Cu

## Results Info



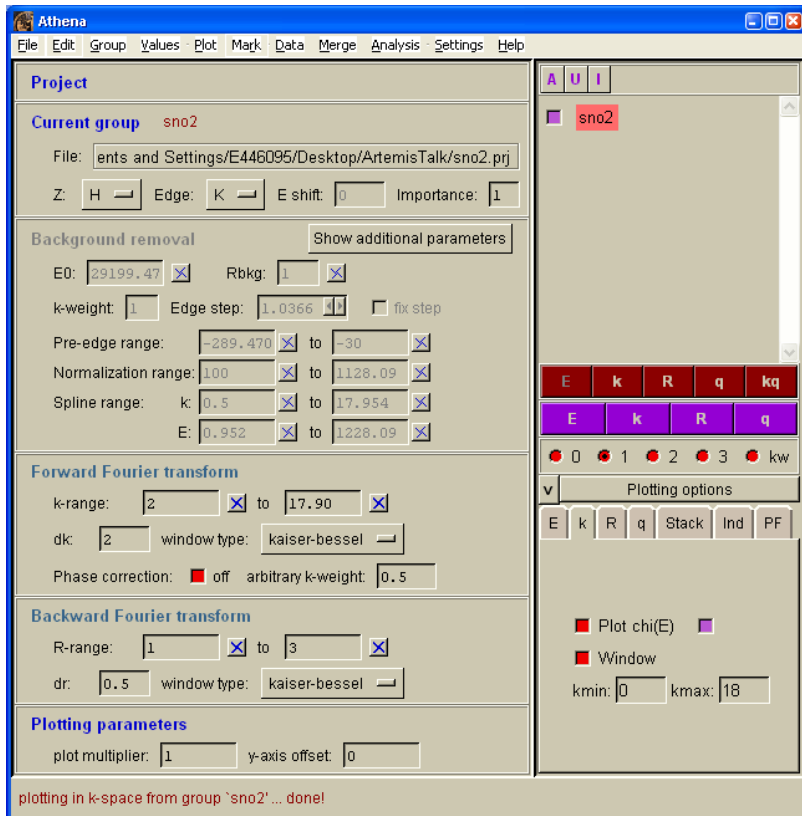
## GSD Info

#	Name	Math Expression
1	g: amp	0.966074 (0.066731)
2	g: enot	5.725481 (0.383385)
3	g: alpha	0.000953 (0.001063)
4	s: temp	10
5	g: theta	286.435582 (41.176460)
6	s: signor	0.00052



- There is more to this example on your computer
- Modeling more shells and modeling temperature dependent spectra series

# Example #2: Align SnO<sub>2</sub> EXAFS Spectra to Theory



**Athena**  
File Edit Group Values Plot Mark Data Merge Analysis Settings Help

**Project**  
Current group: sno2  
File: ents and Settings/E446095/Desktop/ArtemisTalk/sno2.prj  
Z: H Edge: K E shift: 0 Importance: 1

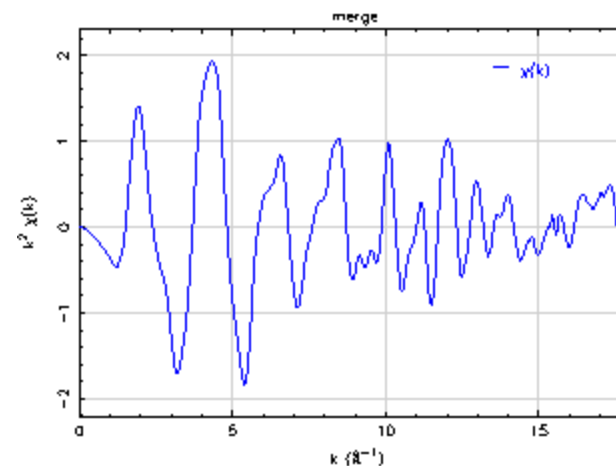
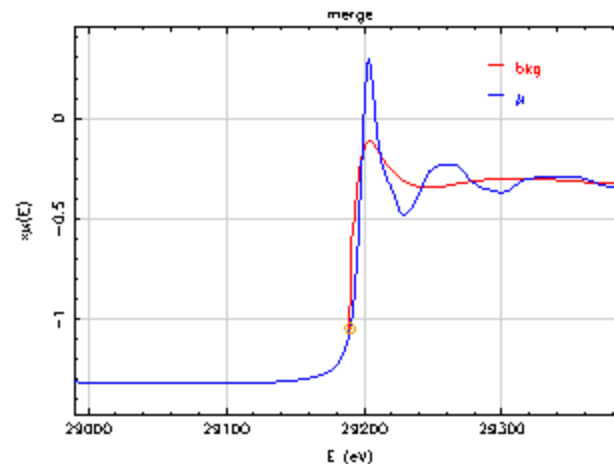
**Background removal** Show additional parameters  
E0: 29199.47 Rbkg: 1  
k-weight: 1 Edge step: 1.0366 fix step  
Pre-edge range: -289.470 to -30  
Normalization range: 100 to 1128.09  
Spline range: k: 0.5 to 17.954 E: 0.952 to 1228.09

**Forward Fourier transform**  
k-range: 2 to 17.90  
dk: 2 window type: kaiser-bessel  
Phase correction: off arbitrary k-weight: 0.5

**Backward Fourier transform**  
R-range: 1 to 3  
dr: 0.5 window type: kaiser-bessel

**Plotting parameters**  
plot multiplier: 1 y-axis offset: 0

plotting in k-space from group 'sno2' ... done!



- E0 is somewhere on the edge
- Using default parameters

M Newville, B Ravel, D Haskel and E A Stern. "Analysis of multiple scattering XAFS data using theoretical standards." *Physica B* 208 & 209: pp 154-156, 1995.

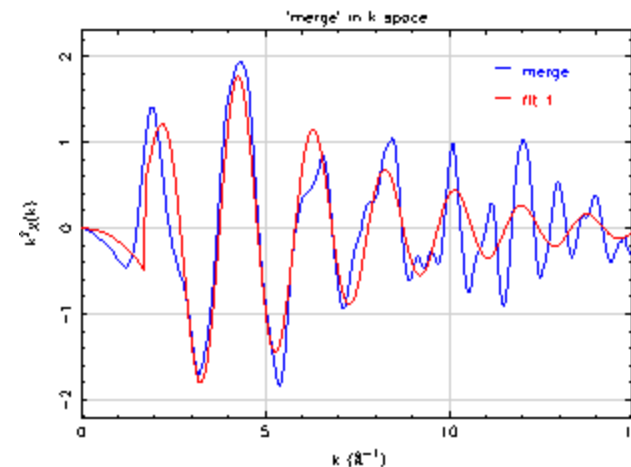
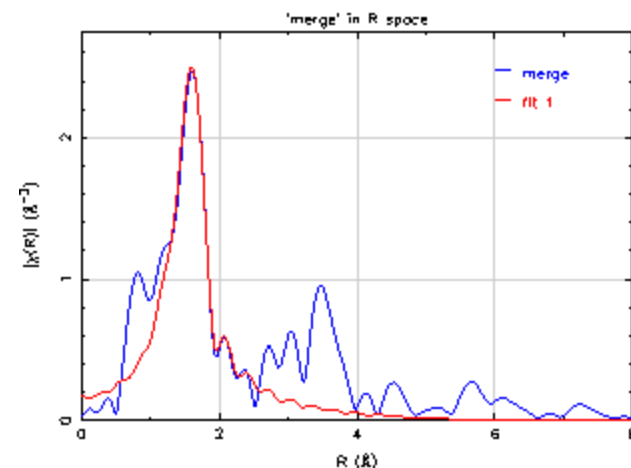
# Fit of first Shell

```
Artemis palettes
|-----|
| fefit | Results | Files | Messages | Echo | Journal | Properties |
|-----|-----|-----|-----|-----|-----|-----|
Results from the last fit
Raw log file | Save | Dismiss
Project title : Fitting chi.chi
Comment       : Fit #1
Prepared by   : skelly@little.er.anl.gov
Contact       :
Started       : 09:28:09 on 11 May, 2004
This fit at   : 14:33:08 on 28 June, 2009
Environment   : Artemis 0.8.013 using Windows XP, perl 5.008008, Tk 804.027, a
Data sets     : "merge"
Fit label     : fit 1
Figure of merit : 1

-----
Independent points      = 12.437500000
Number of variables     = 4.000000000
Chi-square              = 144652.749867735
Reduced Chi-square      = 17144.029613954
R-factor                = 0.063204981
Measurement uncertainty (k) = 0.000180334
Measurement uncertainty (R) = 0.000432656
Number of data sets    = 1.000000000

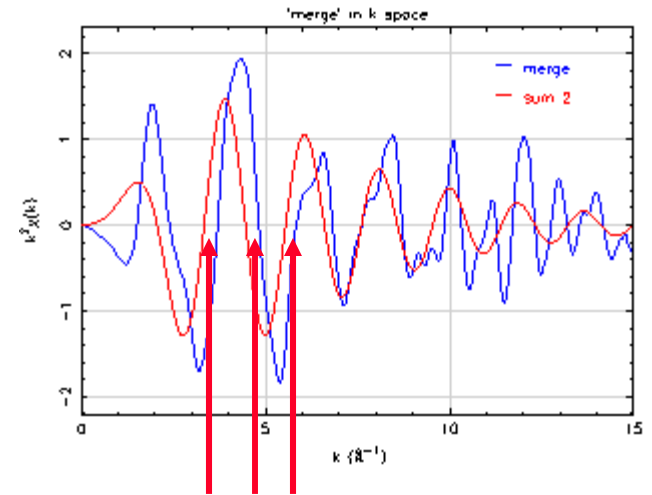
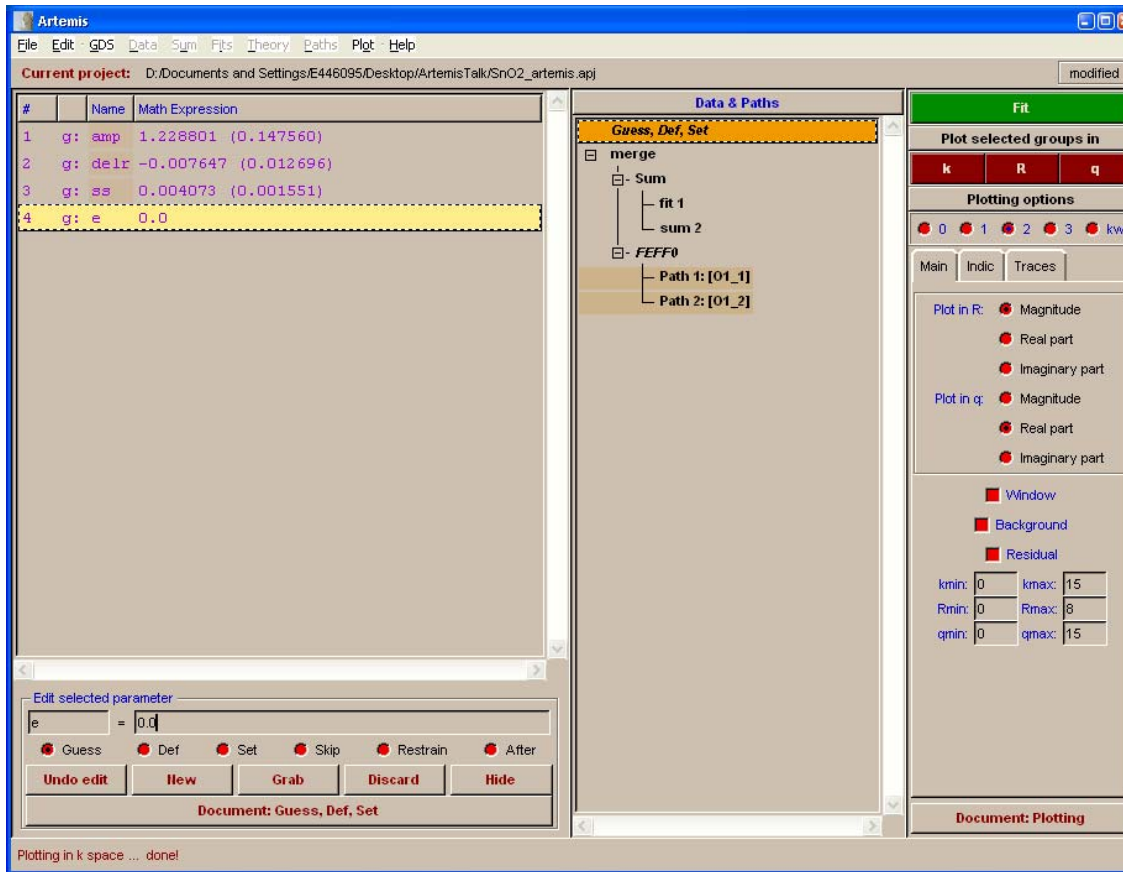
Guess parameters +/- uncertainties (initial guess):
amp      = 1.2288010 +/- 0.1475600 (1.0000)
delr     = -0.0076470 +/- 0.0126960 (0.0000)
ss       = 0.0040730 +/- 0.0015510 (0.0000)
e        = 11.5113960 +/- 1.6084920 (0.0000)

Correlations between variables:
delr and e    --> 0.8451
amp and ss    --> 0.8057
All other correlations are below 0.25
```



- E0 could be smaller
- Background needs to be adjusted
- More information:
- M Newville, B Ravel, D Haskel and E A Stern. "Analysis of multiple scattering XAFS data using theoretical standards." *Physica B* 208 & 209: pp 154-156, 1995.

# Create first shell model with $\Delta E=0$

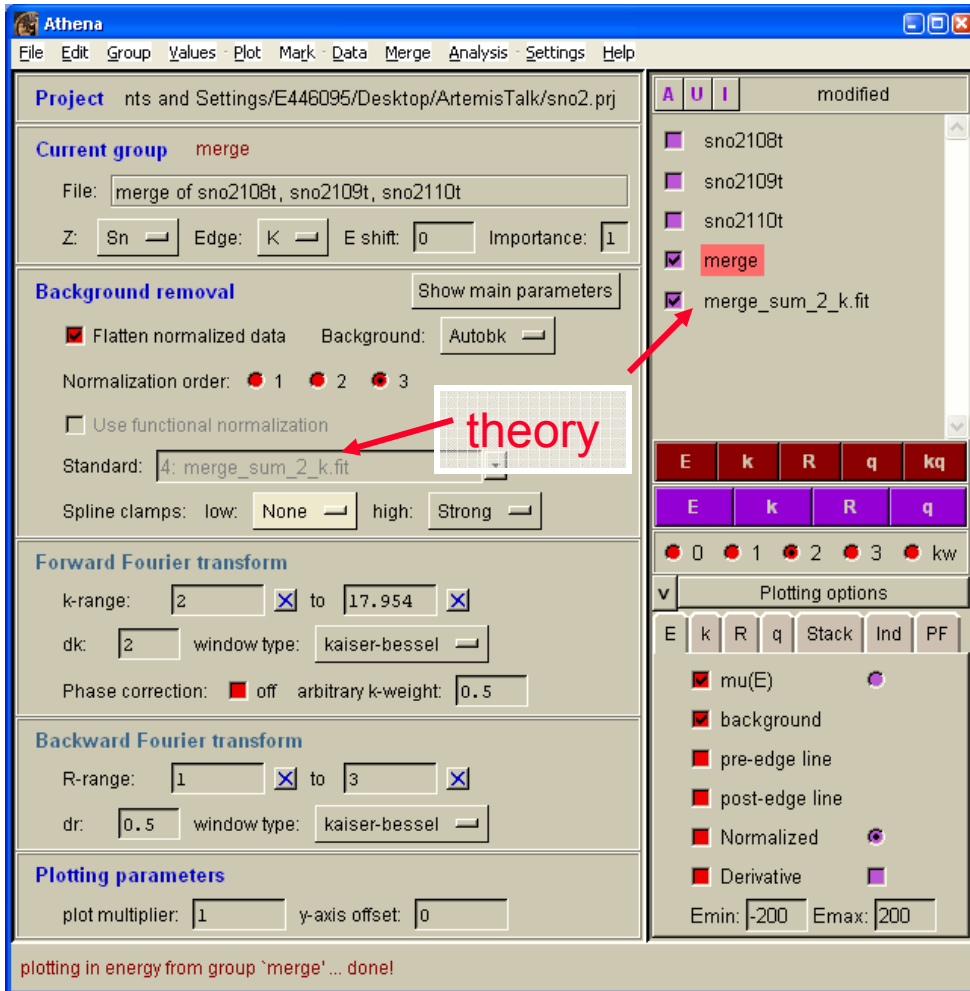
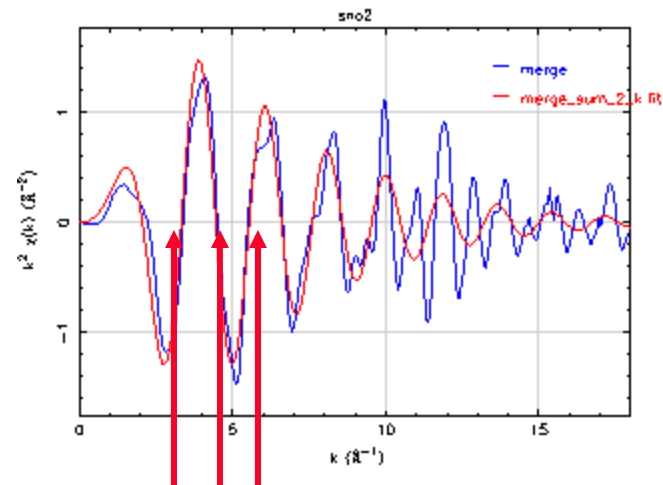
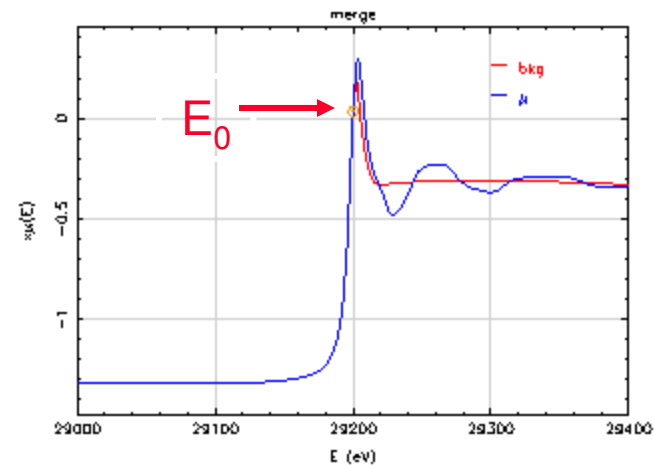


Data and theory are not aligned

- Set parameters to their best-fit values by using the Grab button.
- Set  $e=0$ .
- Sum all paths to make model spectrum with  $E=0$ .



# Background corrected and energy aligned by using theory

Data and theory are aligned

- Read the theory into Athena
- Select your data and use the theory as a standard
- Adjust E0 so that the data and theory are aligned at low k values

# Fit to first shell with background adjusted

Artemis palettes

ifeffit Results Files Messages Echo Journal Properties

Results from the last fit Raw log file Save Dismiss

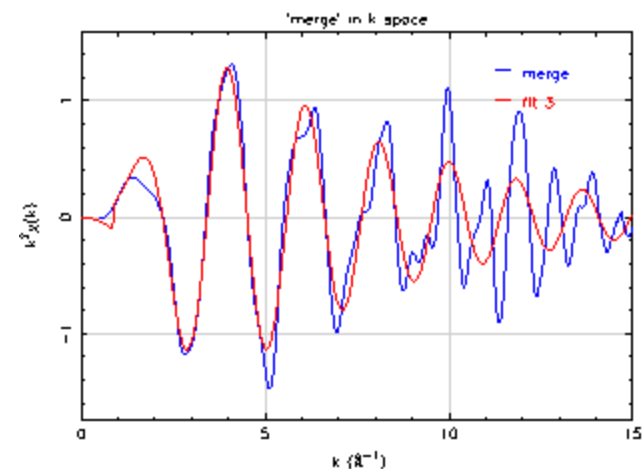
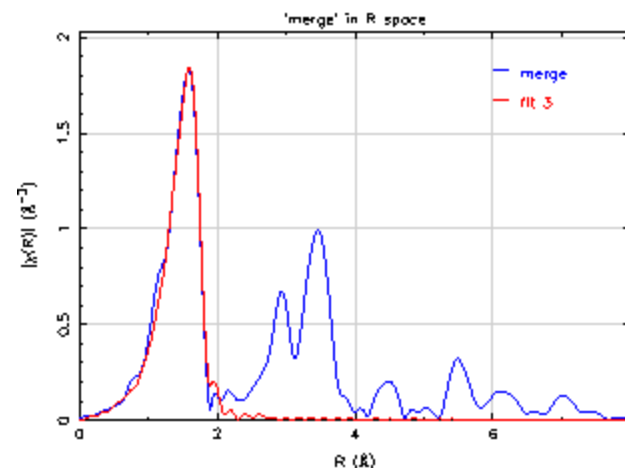
```
Project title : Fitting chi.chi
Comment      : Sum #1
Prepared by  : skelly@little.er.anl.gov
Contact      :
Started      : 09:28:09 on 11 May, 2004
This fit at  : 14:49:08 on 28 June, 2009
Environment  : Artemis 0.8.013 using Windows XP, perl 5.008008, Tk 804.027, a
Data sets    : "merge"
Fit label    : fit 3
Figure of merit : 3

-----

Independent points = 19.875000000
Number of variables = 4.000000000
Chi-square = 7550.041600728
Reduced Chi-square = 475.593171699
R-factor = 0.033932590
Measurement uncertainty (k) = 0.000292358
Measurement uncertainty (R) = 0.001144697
Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):
amp = 0.9586310 +/- 0.0716180 (guessed as 1.228801 (0
delr = -0.0023340 +/- 0.0083500 (guessed as -0.007647 (0
ss = 0.0023830 +/- 0.0010680 (guessed as 0.004073 (0
e = 2.8114190 +/- 0.8594790 (0.0000)

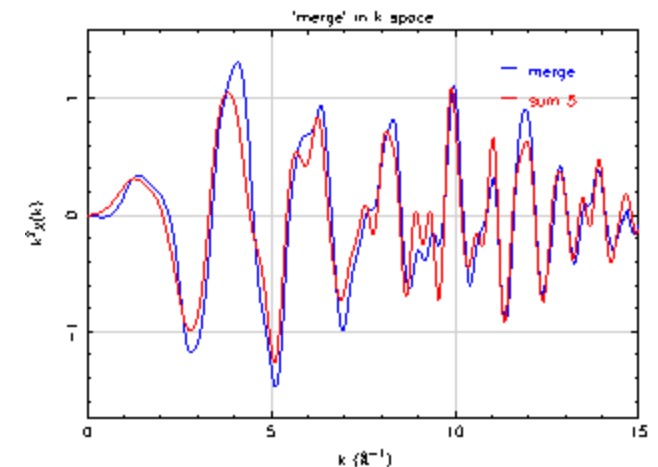
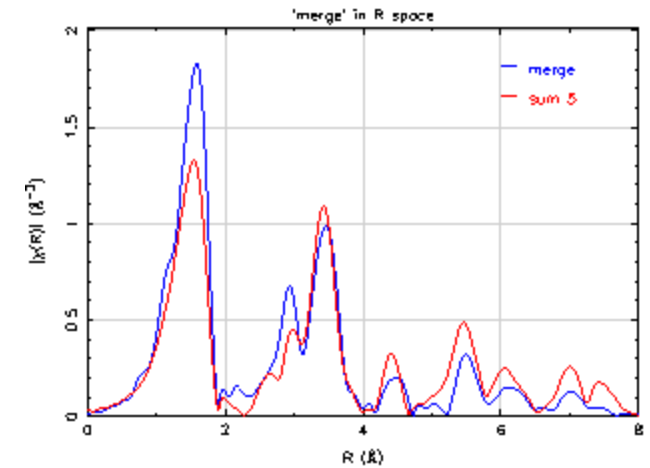
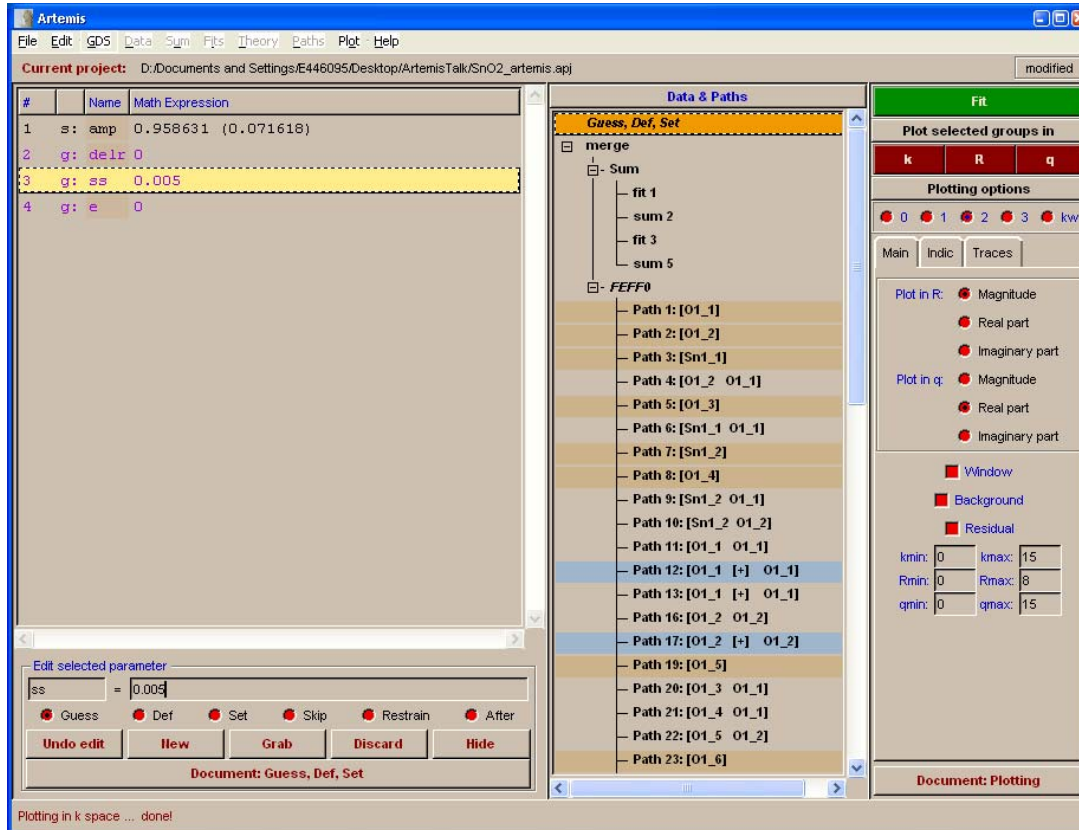
Correlations between variables:
delr and e --> 0.8136
amp and ss --> 0.7698
All other correlations are below 0.25
```



- Read the  $\chi(k)$  data back into Artemis and fit the first shell

# Example 3: Modeling a metal-oxide ( $\text{SnO}_2$ )

- Compare the sum of all 69 paths to the data

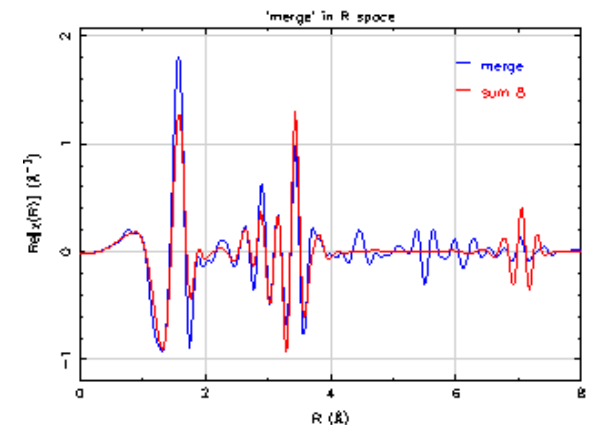
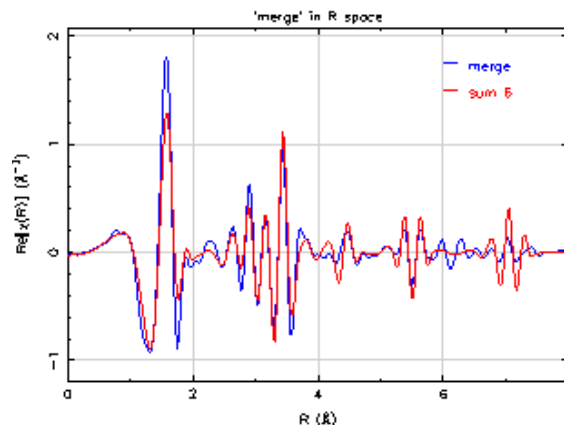
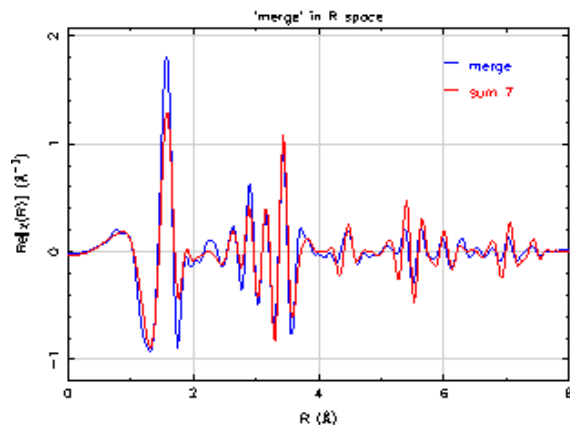
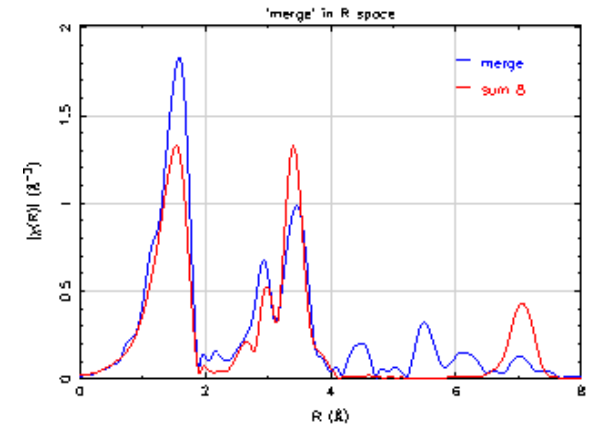
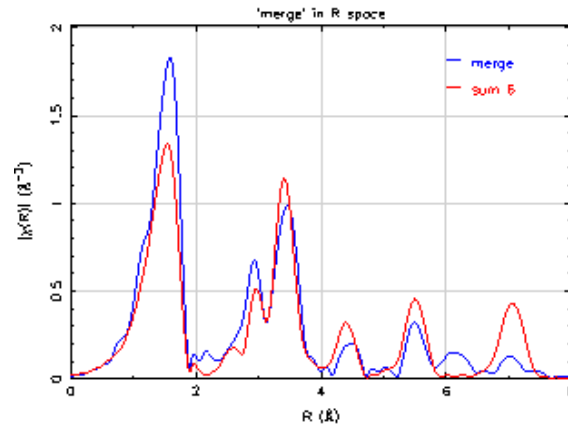
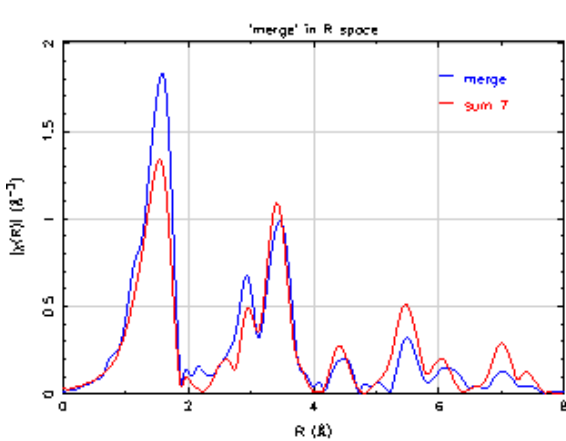


# How many paths are required?

Minimum amplitude 5%  
30 of 69 paths

Minimum amplitude 10%  
18 of 69 paths

Minimum amplitude 15%  
8 of 69 paths



All data is present in model

missing a little of the data

missing a lot of the data

# Models to consider:

- **$\Delta r$ :**
  - Symmetric expansion term: Alpha \* reff.
  - Grouped depending on distance and atom types
  - Related to unit cell dimensions
- **$\Delta E$ :**
  - Energy shifts that depend on atom type
  - One energy shift for all paths
  - Two energy shifts, one for first shell and another for all other shells
- **$\sigma^2$ :**
  - Grouped depending on distance and atom types.
  - Use a Debye or Einstein model, with one or more characteristic temperatures.
  - Each shell with independent value.
  - Separate structural disorder from thermal disorder components.
- **S02:**
  - One S02 for all paths.
  - Approximate S02 from standards.
- **N:**
  - Determined by the crystal structure.
  - Fit a data series were N is expected to change.

# Some EXAFS references

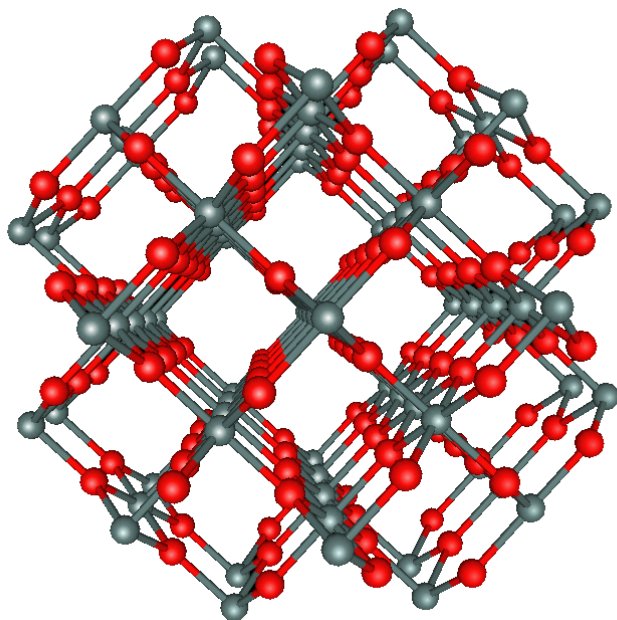
- Multiple edges, structural information: **B Ravel, E. Cockayne, M. Newville and K. M. Rabe.** "Combined EXAFS and first-principles theory study of Pb<sub>1-x</sub>GexTe." Phys. Rev. B 60(21): pp 14632–14642, Dec 1999
- Structural information, bond angles: **A. I. Frenkel, E A Stern, A. Voronel, M. Qian and M Newville.** "Solving the structure of disordered mixed salts." Phys. Rev. B 49(17 – 1): pp 11662–11674, May 1994.
- Model two phases, then combined to model a mixture: **S. Kelly, R. Ingalls, F. Wang, B. Ravel and D. Haskel.** "X-ray-absorption fine-structure study of the B1-to-B2 phase transition in RbCl." Phys. Rev. B 57(13): pp 7543–7550, April 1998
- Determine neighbor atom types and number using standards: **S. D. Kelly, K. M. Kemner, J. B. Fein, D. A. Fowle, M. I. Boyanov, B. A. Bunker and N. Yee.** "X-ray absorption fine-structure determination of pH dependent U-bacterial cell wall interactions." Geochem. Cosmo. acta. 66(22): pp 3855-3871, Nov 2002.
- Multiple techniques: **P G Allen, J J Bucher, D L Clark, N M Edelstein, S A Ekberg, J W Gohdes, E A Hudson, N Kaltsoyannis, W W Lukens, M P Neu, P D Palmer, T Reich, D K Shuh, C D Tait and B D Zwick.** "Multinuclear NMR, Raman, EXAFS, and X-ray diffraction studies of uranyl carbonate complexes in near-neutral aqueous solution. X-ray structure of [C(NH<sub>2</sub>)<sub>3</sub>]<sub>6</sub>[(UO<sub>2</sub>)<sub>3</sub>(CO<sub>3</sub>)<sub>6</sub>] 6.5H<sub>2</sub>O." Inorg. Chem. 34: pp 4797-4807, 1995.
- Pressure dependent data: **A. I. Frenkel, F. M. Wang, S. Kelly, R. Ingalls, D. Haskel, E. A. Stern and Y. Yacoby,** "Local structural changes in KNbO<sub>3</sub> under high pressure", *Physical Review B* 56, 10869, 1997.
- Temperature dependent data: **D. Haskel, E.A. Stern, D.G. Hinks, A.W. Mitchell, J.D. Jorgensen, J.I. Budnick,** "Dopant and Temperature Induced Structural Phase Transitions in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub>" *Physical Review Letters*, 76 (3) pg 439
- Multiple edges, structural disorder: **S. Calvin, E. E. Carpenter, B. Ravel, V. G. Harris and S. A. Morrison.** "Multiedge refinement of extended x-ray-absorption fine structure of manganese zinc ferrite nanoparticles." Phys. Rev. B 66: pp 224405, 2002.
- Structural information from XANES and EXAFS: **B. Ravel, E. A. Stern, R. I. Vedrinskii and V. Kraizman.** "Local structure and the phase transitions of BaTiO<sub>3</sub>." FERROELECTRICS 206(1-4): pp 407-430, 1998.
- Temperature dependence and nanoparticles: **A. I. Frenkel, C. W. Hills and R. G. Nuzzo.** "A view from the inside: Complexity in the atomic scale ordering of supported metal nanoparticles." JOURNAL OF PHYSICAL CHEMISTRY B 105(51): pp 12689-12703, 2001.
- **Kelly, S. D.; Hesterberg, D.; Ravel, B.** Analysis of soils and minerals using X-ray absorption spectroscopy. In *Methods of soil analysis, Part 5 -Mineralogical methods*; Ulery, A. L., Drees, L. R., Eds.; Soil Science Society of America: Madison, WI, USA, 2008; pp 367-463.

# The Model for SnO<sub>2</sub> data

- **$\Delta r$** : symmetric expansion term:  $\alpha * \text{reff}$ .
- **$\Delta E$** : Energy shifts that depend on atom type:
  - The first shell; Eo1,
  - All other oxygen scattering events: Eo2
  - All tin scattering events: Esn
- **$\sigma^2$** : Grouped depending on distance and atom types.
- **$S_0^2$** : one for all paths.
- **N**: determined from the crystal structure.

# Final Model for SnO<sub>2</sub>

Includes all the  
atoms shown here

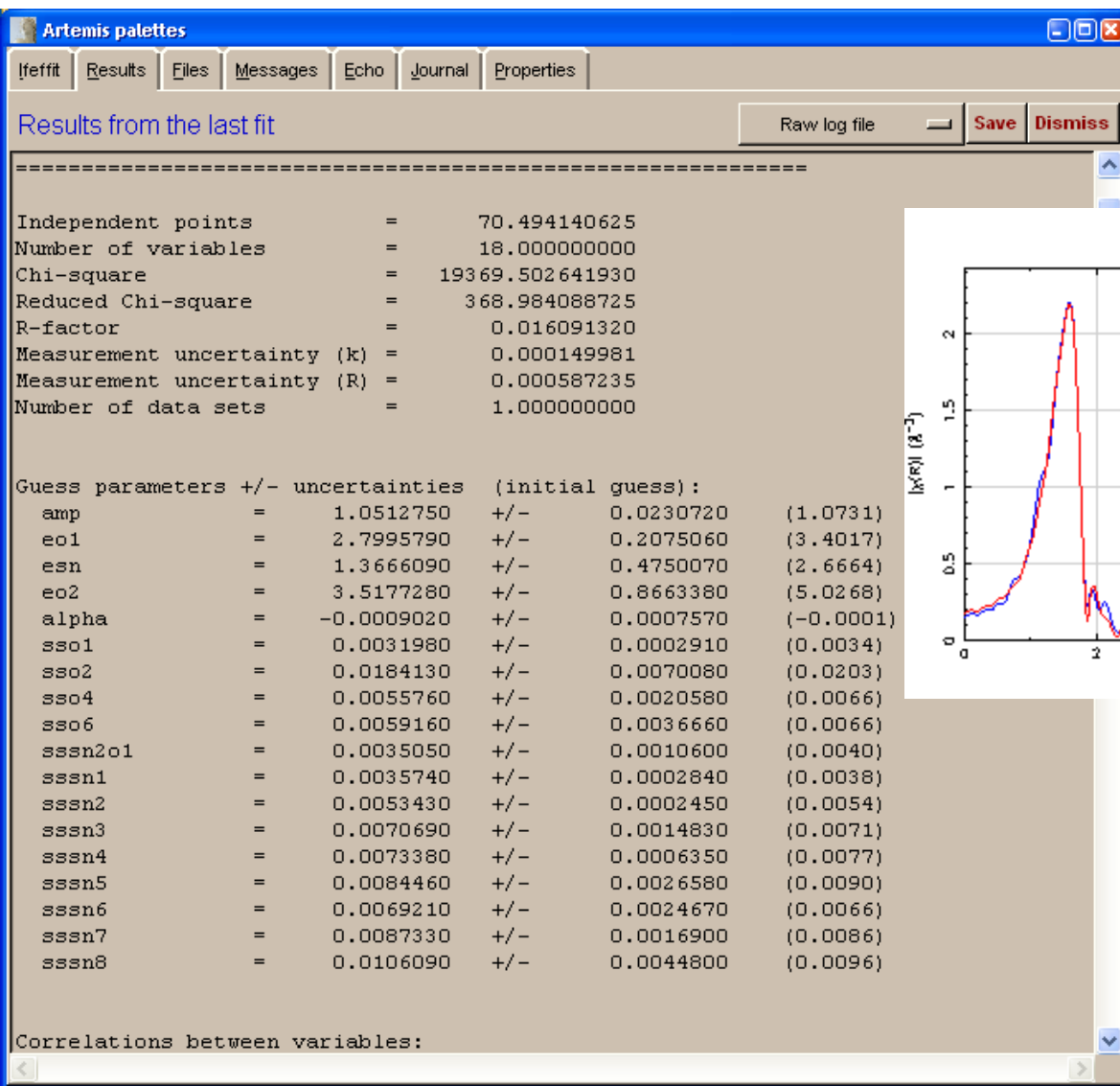


<i>Path</i>	<i>N</i>	<i>reff</i>	$\Delta R$	$\sigma^2$	$\Delta E$
Sn-O1	4	2.0519	Alpha-ref	$\sigma^2_{o1}$	$\Delta E_{o1}$
Sn-O2	2	2.0567	Alpha-ref	$\sigma^2_{o1}$	$\Delta E_{o1}$
Sn-Sn1	2	3.1864	Alpha-ref	$\sigma^2_{sn1}$	$\Delta E_{sn}$
Sn-O3	4	3.5906	Alpha-ref	$\sigma^2_{o3}$	$\Delta E_{o2}$
Sn-Sn2	8	3.7093	Alpha-ref	$\sigma^2_{sn2}$	$\Delta E_{sn}$
Sn-Sn2-O1	8	3.9090	Alpha-ref	$\sigma^2_{sn2o1}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn2-O2	8	3.9090	Alpha-ref	$\sigma^2_{sn2o1}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-O5	8	4.2414	Alpha-ref	$\sigma^2_{o5}$	$\Delta E_{o2}$
Sn-Sn3	4	4.7373	Alpha-ref	$\sigma^2_{sn3}$	$\Delta E_{sn}$
Sn-O7	8	4.8006	Alpha-ref	$\sigma^2_{o7}$	$\Delta E_{o2}$
Sn-Sn4	8	5.7092	Alpha-ref	$\sigma^2_{sn4}$	$\Delta E_{sn}$
Sn-Sn5	8	5.8365	Alpha-ref	$\sigma^2_{sn4}$	$\Delta E_{sn}$
Sn-Sn5-O1	8	5.8405	Alpha-ref	$\sigma^2_{sn4}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn5-O4	8	5.8405	Alpha-ref	$\sigma^2_{sn4}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o2}$
Sn-O1-Sn5-O1	4	5.8444	Alpha-ref	$\sigma^2_{sn4}$	$0.33 \cdot \Delta E_{sn} + 0.66 \cdot \Delta E_{o1}$
Sn-O4-Sn5-O4	4	5.8444	Alpha-ref	$\sigma^2_{sn4}$	$0.33 \cdot \Delta E_{sn} + 0.66 \cdot \Delta E_{o2}$
Sn-Sn6-Sn1	4	6.3728	Alpha-ref	$\sigma^2_{sn6}$	$\Delta E_{sn}$
Sn-Sn1-Sn6-Sn1	2	6.3728	Alpha-ref	$\sigma^2_{sn6}$	$\Delta E_{sn}$
Sn-Sn7	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$\Delta E_{sn}$
Sn-Sn7-O2	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn7-O6	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o2}$
Sn-Sn7-O6-O2	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.33 \cdot \Delta E_{sn} + 0.33 \cdot \Delta E_{o1} + 0.33 \cdot \Delta E_{o2}$
Sn-O6-Sn7-O2	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.33 \cdot \Delta E_{sn} + 0.33 \cdot \Delta E_{o1} + 0.33 \cdot \Delta E_{o2}$
Sn-O2-Sn7-O6-O2	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.25 \cdot \Delta E_{sn} + 0.50 \cdot \Delta E_{o1} + 0.25 \cdot \Delta E_{o2}$
Sn-O6-Sn7-O6-O2	4	6.6995	Alpha-ref	$\sigma^2_{sn7}$	$0.25 \cdot \Delta E_{sn} + 0.25 \cdot \Delta E_{o1} + 0.50 \cdot \Delta E_{o2}$
Sn-Sn8	8	7.4187	Alpha-ref	$\sigma^2_{sn8}$	$\Delta E_{sn}$
Sn-Sn8-Sn2	16	7.4187	Alpha-ref	$\sigma^2_{sn8}$	$\Delta E_{sn}$
Sn-Sn2-Sn-Sn2	8	7.4187	Alpha-ref	$4 \cdot \sigma^2_{sn2}$	$\Delta E_{sn}$
Sn-Sn2-Sn8-Sn2	8	7.4187	Alpha-ref	$\sigma^2_{sn8}$	$\Delta E_{sn}$
Sn-Sn9	16	7.6578	Alpha-ref	$\sigma^2_{sn9}$	$\Delta E_{sn}$

- One S02-value was also determined in the fit.
- 30 paths used in final model.
- There are a total of 18 parameters in this model and 56 independent points in the data.



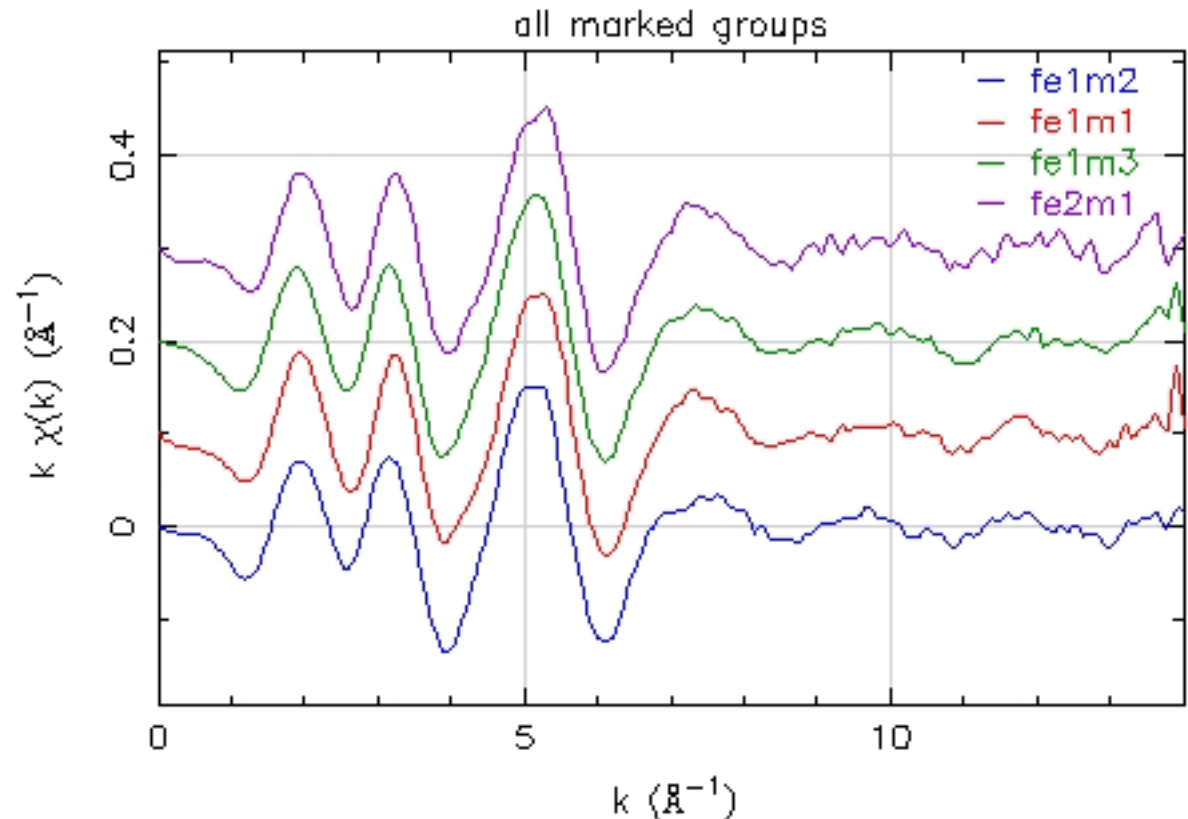
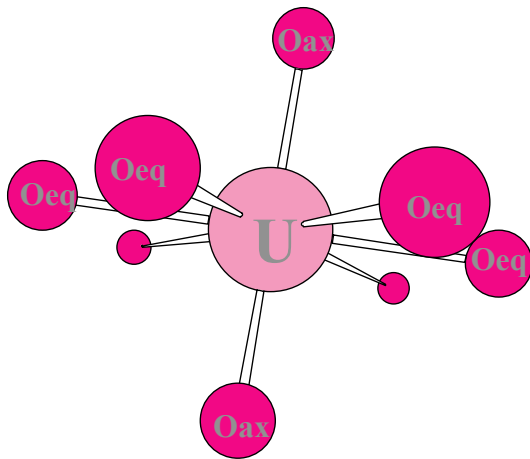
# Final Model and Fit to SnO<sub>2</sub>



- Typical values for EXAFS parameters
- $\Delta r$ : less than 0.5 Å
- $\Delta E$ : less than 10 eV
- $\sigma^2$ : 0.003 to 0.020 Å<sup>2</sup>
- S02: 0.70 to 1.10

# Example 4: Determining 2<sup>nd</sup> shell atom type and number

- Uranyl in equilibrium with a mixture of Fe-oxides and different microbial components.
- Possible second shell atoms, O, C, P, Fe, U.
- 30-50 combinations of these atoms were tested.
- Three of these tests are shown here:
  - C and Fe,
  - P and Fe,
  - Fe and Fe



# Setting up a Uranyl Model

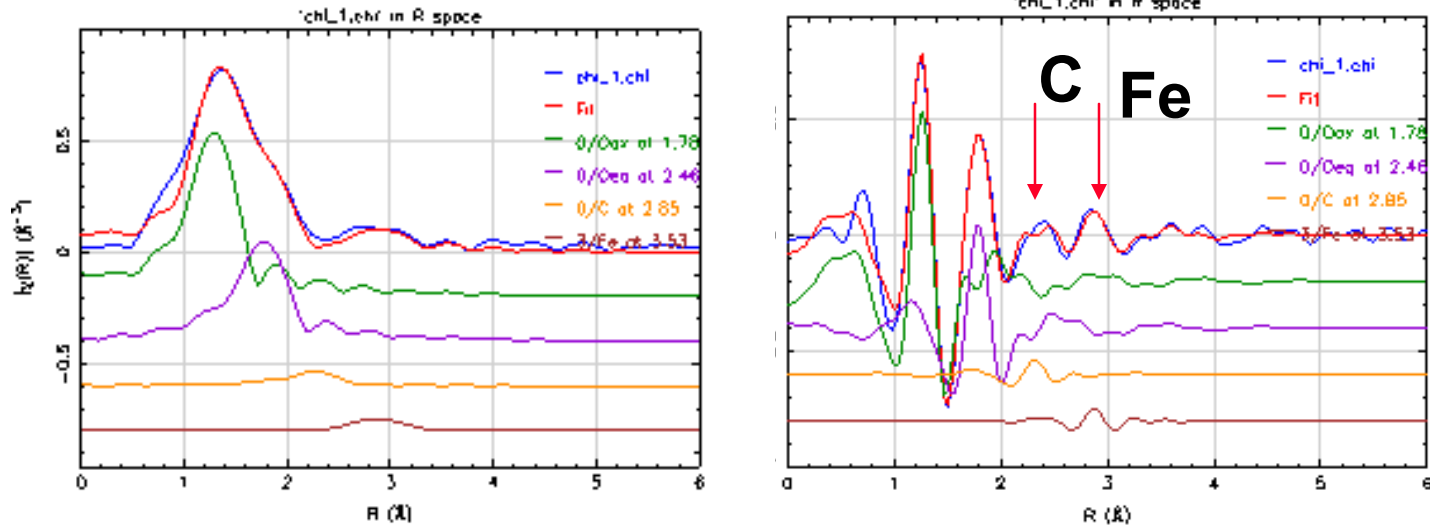
The screenshot shows the Artemis software interface. The main window is titled 'Artemis' and has a menu bar with 'File', 'Edit', 'GDS', 'Data', 'Sym', 'Plts', 'Theory', 'Paths', 'Plot', and 'Help'. The current project is 'D:/Documents and Settings/E446095/Desktop/ArtemisTalk/artemis1-TestPaths.apj'. The interface is divided into several panels:

- Table:** A table with columns '#', 'Name', and 'Math Expression'. It lists parameters like 'g: noeq', 'g: deloeq', 'g: ssoeq', 'g: nfe2', 'g: delfe2', 'd: ssfe2', 'g: nc', 'g: delc', 'g: ssc', 'np', 'delp', 'ssp', 'nfe1', 'delfe1', and 'ssfe1'.
- Data & Paths:** A tree view showing the model structure. It includes 'chi\_1.chi', 'Fit', 'FEFF0', 'FEFF1', 'FEFF3', and 'FEFF4'. Each FEFF path has associated parameters like 'Oax at 1.78', 'Oeq at 2.46', 'C at 2.85', 'P at 3.06', and 'Fe at 3.53'.
- Fit:** A panel for fitting the model. It has a 'Fit' button, a 'Plot selected groups in' section with buttons for 'k', 'R', and 'q', and 'Plotting options' for '0', '1', '2', '3', and 'kw'. It also has tabs for 'Main', 'Indic', and 'Traces'.
- Edit selected parameter:** A panel for editing the selected parameter 'ssp'. It shows 'ssp = 0.003' and buttons for 'Guess', 'Def', 'Set', 'Skip', 'Restrained', and 'After'. There are also buttons for 'Undo edit', 'New', 'Grab', 'Discard', and 'Hide'.

At the bottom of the window, it says 'Document: Guess, Def, Set' and 'ssp = -0.000673 +/- 0.019959'.

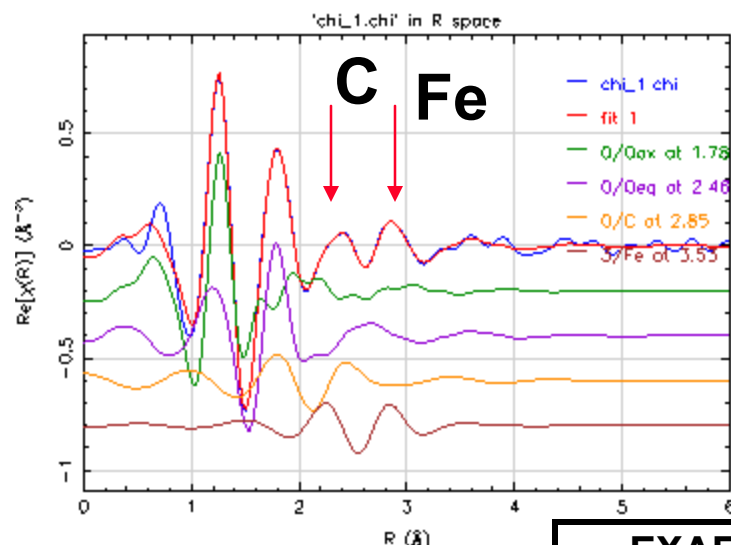
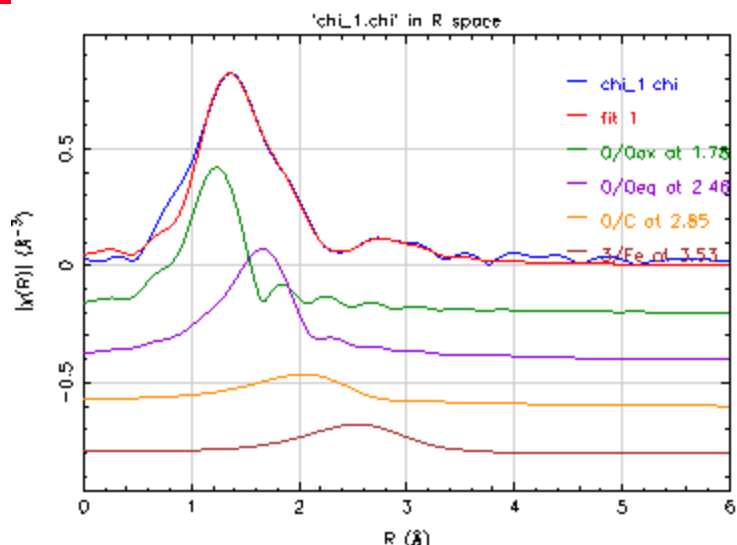
- Organization is key
- FEFF paths can be renamed
- Separators can be added to GDS page
- Variable names can have meaning
- Multiple FEFF calculations can be used in one model

# Test data for C and Fe shells



- Place **C** and **Fe** shells in a “good” spot
  - set parameters – no fitting
  - monitor results and fit spectra
  - Needs to be done using real or imaginary part of FT, can not always be done using magnitude of FT.

# Fit Results using C and Fe shells



Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

Results from the last fit

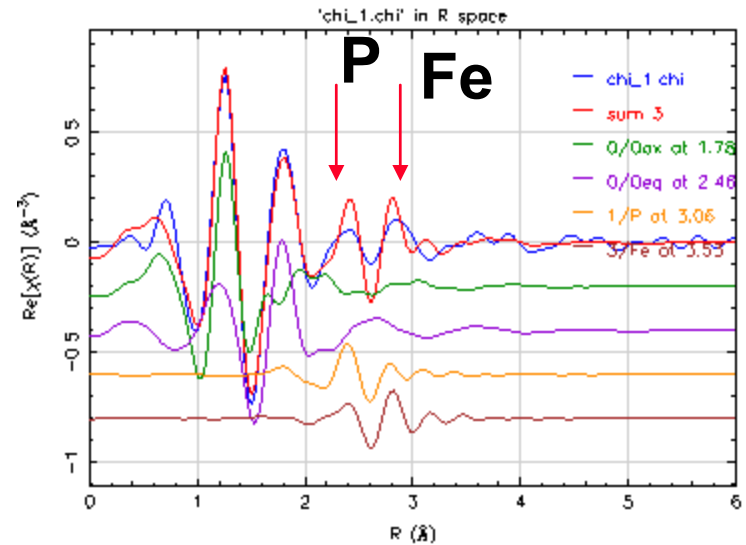
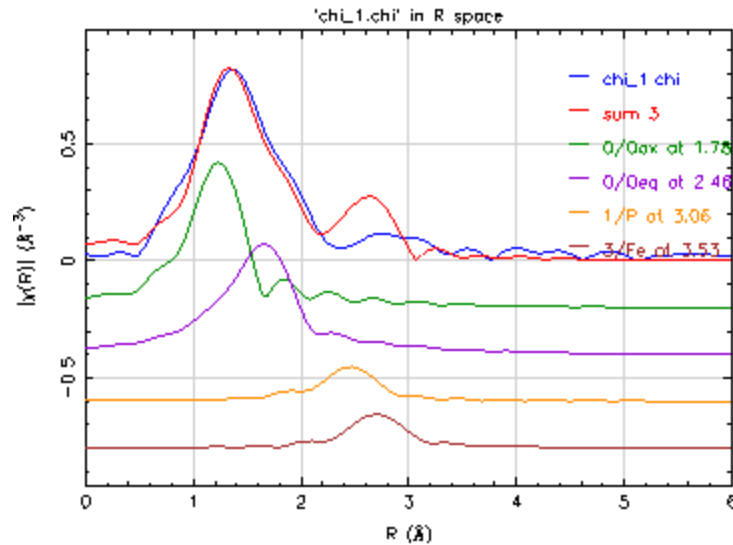
R-factor for this data set = 0.00203

path	degen	amp	sigma <sup>2</sup>	e0	reff	delta_R	R
"FEFF0: Oax at 1.78"	1.00000	2.000	0.00386	-8.79362	1.75510	-0.00517	1.74993
"FEFF0: Oeq at 2.46"	1.00000	5.719	0.01094	-8.79362	2.46160	-0.21986	2.24174
"FEFF0: C at 2.85"	1.00000	21.896	0.03066	-8.79362	2.85250	0.01219	2.86469
"FEFF0: U-Oax1-U-Oax1"	1.00000	2.000	0.01546	-8.79362	3.51020	-0.01035	3.49985
"FEFF0: U-Oax1-Oax2"	1.00000	2.000	0.00773	-8.79362	3.51580	-0.01035	3.50545
"FEFF0: U-Oax1-U-Oax2"	1.00000	2.000	0.00386	-8.79362	3.51580	-0.01035	3.50545
"FEFF3: Fe at 3.53"	1.00000	20.066	0.03957	-8.79362	3.52570	-0.26212	3.26358

EXAFS Parameters	
$\sigma^2$ -values	-
Distances	+
Coordination numbers	-
$\Delta E$ -value	-

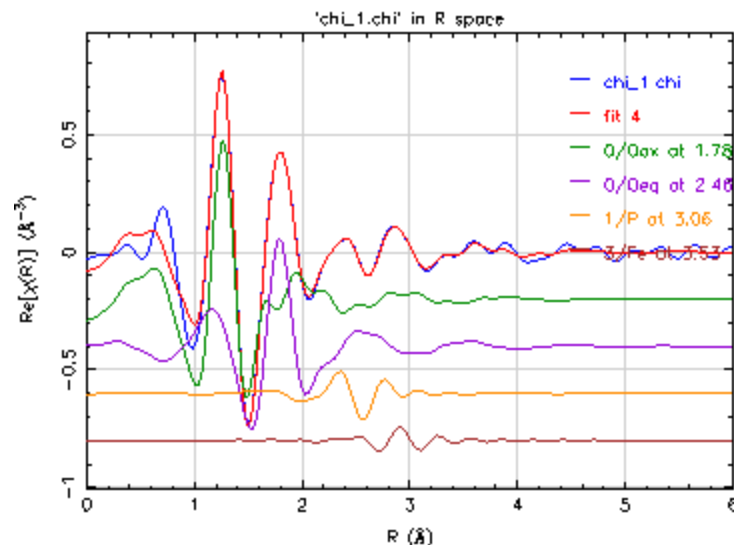
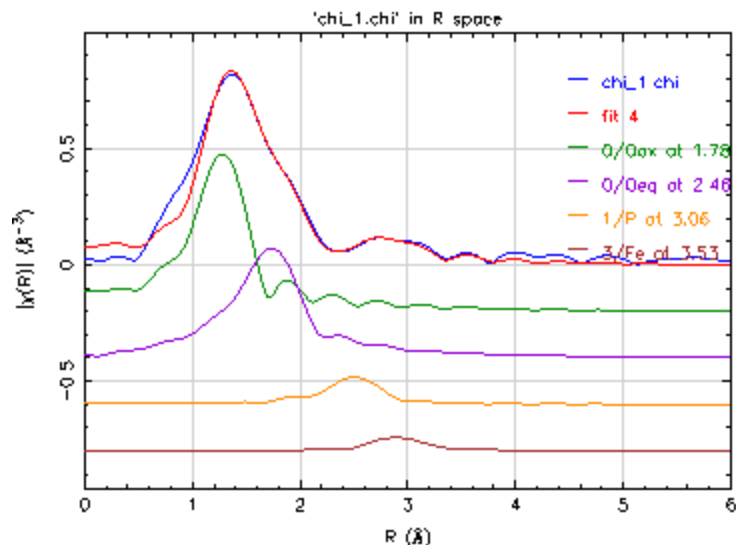
Signals became broad and unrealistic

# Test data for P and Fe shells



- Place **P** and **Fe** shells in a “good” spot
  - set parameters – no fitting
  - monitor results and fit spectra

# Fit Results using P and Fe shells



Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

Results from the last fit

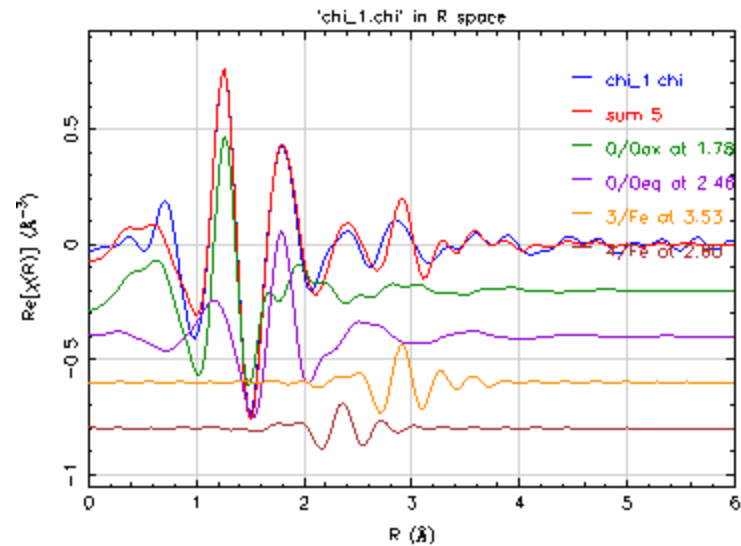
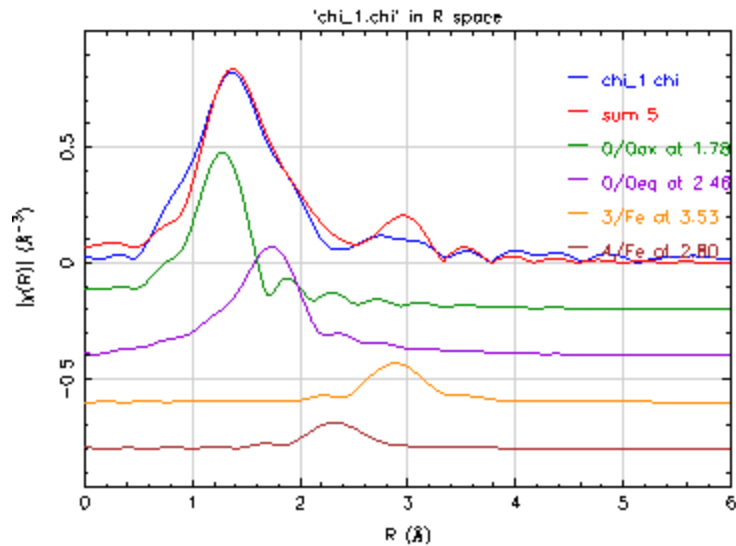
R-factor for this data set = 0.00264

path	degen	amp	sigma <sup>2</sup>	e0	reff	delta_R	R
"FEFF0: Oax at 1.78"	1.00000	2.000	0.00351	-1.12310	1.75510	0.02066	1.77576
"FEFF0: Oeq at 2.46"	1.00000	4.615	0.00941	-1.12310	2.46160	-0.17609	2.28551
"FEFF0: U-Oax1-U-Oax1"	1.00000	2.000	0.01405	-1.12310	3.51020	0.04132	3.55152
"FEFF0: U-Oax1-Oax2"	1.00000	2.000	0.00702	-1.12310	3.51580	0.04132	3.55712
"FEFF0: U-Oax1-U-Oax2"	1.00000	2.000	0.00351	-1.12310	3.51580	0.04132	3.55712
"FEFF1: P at 3.06"	1.00000	0.835	0.00398	-1.12310	3.05550	0.00987	3.06537
"FEFF3: Fe at 3.53"	1.00000	0.276	0.00139	-1.12310	3.52570	-0.12876	3.39694

## EXAFS Parameters

$\sigma^2$ -values	-
Distances	+
Coordination numbers	+
$\Delta E$ -value	+

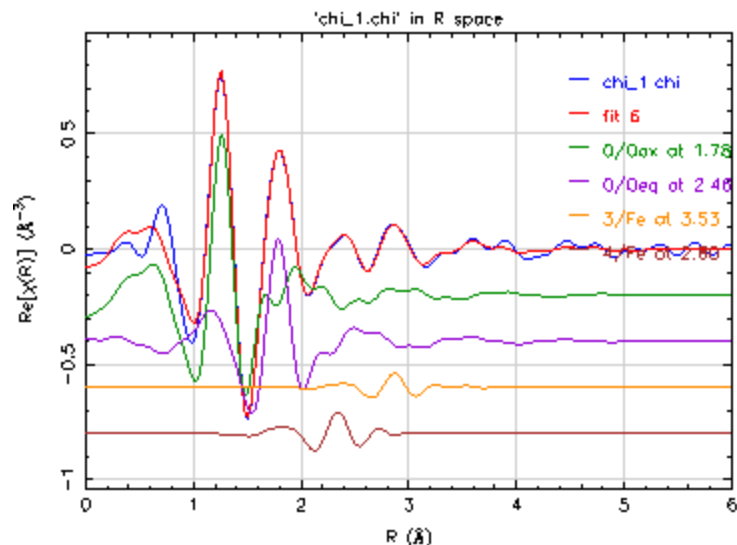
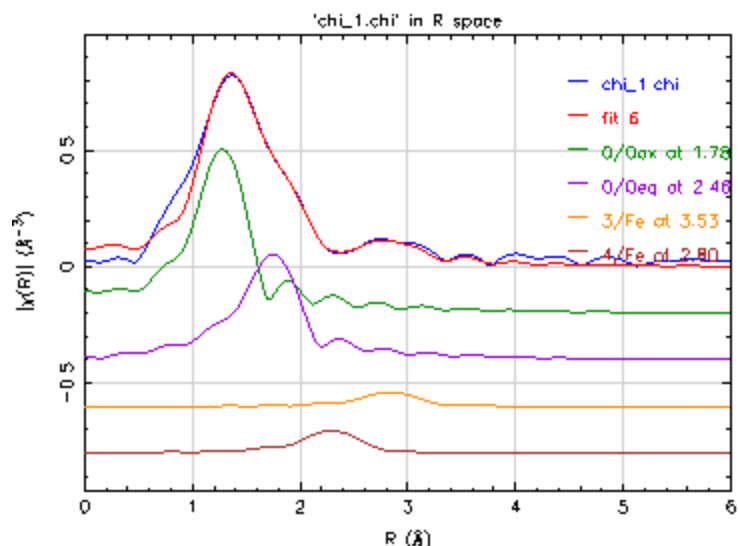
# Test data for Fe and Fe shells



- **Place Fe and Fe shells in a “good” spot**
  - set parameters – no fitting
  - monitor results and fit spectra



# Fit Results using Fe and Fe shells



Artemis palettes

Results from the last fit

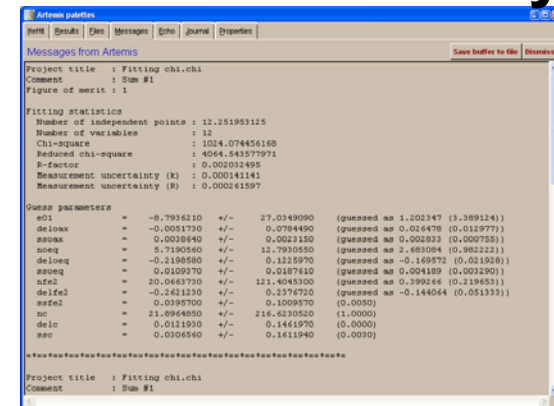
R-factor for this data set = 0.00254

path	degen	amp	sigma <sup>2</sup>	e0	reff	delta_R	R
"FEFF0: Oax at 1.78"	1.00000	2.000	0.00320	-0.59470	1.75510	0.01998	1.77508
"FEFF0: Oeq at 2.46"	1.00000	3.235	0.00594	-0.59470	2.46160	-0.17897	2.28263
"FEFF0: U-Oax1-U-Oax1"	1.00000	2.000	0.01280	-0.59470	3.51020	0.03995	3.55015
"FEFF0: U-Oax1-Oax2"	1.00000	2.000	0.00640	-0.59470	3.51580	0.03995	3.55575
"FEFF0: U-Oax1-U-Oax2"	1.00000	2.000	0.00320	-0.59470	3.51580	0.03995	3.55575
"FEFF3: Fe at 3.53"	1.00000	0.670	0.00830	-0.59470	3.52570	-0.16117	3.36453
"FEFF4: Fe at 2.80"	1.00000	0.669	0.00830	-0.59470	2.80090	0.03782	2.83872

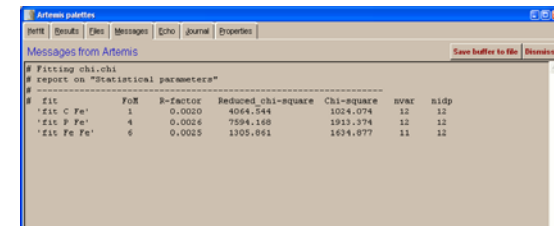
EXAFS Parameters	
$\sigma^2$ -values	+
Distances	+
Coordination numbers	+
$\Delta E$ -value	+

# Comparison of Models

## Quick summary



## Parameter Report



Artemis  
File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: D:\Documents and Settings\E446095\Desktop\ArtemisTalk\artemis1-TestPaths.apj

Examine log files  
Current fit: fit Fe Fe

Fits  
fit C Fe  
sum 2  
sum 3  
fit P Fe  
sum 5  
fit Fe Fe

Choose a parameter  
Statistical parameters  
Get parameters from Guess, Def, Set list

Parameter report

Calculations  
 Compute the average value  
 Fit Einstein temp. to sigma^2 values  
Absorber:  Scatterer:   
 Prefer R-factor  
 Prefer reduced chi-square  
 Show y=0 in plot

Quick summaries of selected fits

Select all  
Clear selection

Document: Log viewer

Data & Paths  
Guess, Def, Set  
chi\_1.chi  
Fit  
fit C Fe  
sum 2  
sum 3  
fit P Fe  
sum 5  
fit Fe Fe  
FEFF0  
Oax at 1.78  
Oeq at 2.46  
C at 2.85  
U-Oax1-U-Oax1  
U-Oax1-Oax2  
U-Oax1-U-Oax2  
FEFF1  
P at 3.06  
FEFF3  
Fe at 3.53  
FEFF4  
Fe at 2.80

Fit  
Plot selected groups in  
k R q  
Plotting options  
0 1 2 3 kw  
Main Indic Traces  
Plot in R:  Magnitude  
 Real part  
 Imaginary part  
Plot in q:  Magnitude  
 Real part  
 Imaginary part  
 Window  
 Background  
 Residual  
kmin: 0 kmax: 15  
Rmin: 0 Rmax: 6  
qmin: 0 qmax: 15

Document: Plotting

Loaded parameter list from GDS page

- Models are saved in Artemis and can be compared or re-instated later

# Multiple data set fit

Common variables for all 4 data sets

variables for each data set

The screenshot shows the Artemis software interface with the following components:

- Variable List (Left):** A table with columns for variable name and math expression.
 

#	Name	Math Expression
1	s: amp	1.0
2	s: de1oax	0.014617 (0.013632)
3	s: ssoax	0.002837 (0.000787)
4	s: noe1	3.216381 (1.490651)
5	s: de1oeq	-0.181129 (0.025391)
6	s: ssoeq	0.006175 (0.004317)
7	g: delife1	0.037073 (0.036027)
8	g: ssfe1	0.003715 (0.007244)
9	g: delife2	-0.165025 (0.047100)
10	d: ssfe2	ssfe1
11	---	---
12	g: nfe1a	0.491382 (0.415475)
13	g: nfe1b	0.459836 (0.414836)
14	g: nfe1c	0.579083 (0.463117)
15	g: nfe1d	0.452179 (0.390209)
16	g: nfe2a	0.511882 (0.491440)
17	g: nfe2b	0.472358 (0.519707)
18	g: nfe2c	0.392737 (0.514444)
19	g: nfe2d	0.663336 (0.658349)
- Data & Paths (Middle):** A tree view showing the fit structure for two data sets:
  - chi\_1.chi
    - Fit
    - FEFF0
      - Oax at 1.76
      - Oeq at 2.46
      - U-Oax1-U-Oax1
      - U-Oax1-U-Oax2
    - FEFF1
    - FEFF18
    - FEFF3
      - Fe at 3.53
    - FEFF4
      - Fe at 2.80
  - chi\_2.chi
    - Fit
    - FEFF14
      - Fe at 3.53
    - FEFF17
    - FEFF5
      - Oax at 1.76
      - Oeq at 2.46
      - U-Oax1-U-Oax1
      - Oax1-U-Oax2
    - FEFF7
      - Fe at 2.80
- Fit (Right):** Configuration for the fit, including:
  - Plot selected groups in: k, R, q
  - Plotting options: Magnitude, Real part, Imaginary part for both k and q.
  - Window, Background, Residual checkboxes.
  - Range sliders: kmin: 0, kmax: 15; Rmin: 0, Rmax: 10; qmin: 0, qmax: 15.

Data set 1

Data set 2

- Fit 4 data sets
- Use K-weights of 1, 2 and 3
- Fit different N values for each data set
- Data series is needed to accurately determine the number of Fe atoms in the 2<sup>nd</sup> and 3<sup>rd</sup> shells

# Modeling a Data Series

Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

Results from the last fit

Environment : Artemis 0.8.013 using Windows XP, perl 5.008008, Tk 8.0  
 Fit label : fit Fe Fe  
 Data sets : "chi\_1.chi", "chi\_2.chi", "chi\_3.chi", "chi\_4.chi"  
 Figure of merit : 7

---

Fitting statistics

Number of independent points : 26.578125000  
 Number of variables : 11  
 Chi-square : 9490.351885016  
 Reduced chi-square : 609.210151094  
 R-factor : 0.057174889  
 Measurement uncertainty (k) : 0.000196055  
 Measurement uncertainty (R) : 0.000220316

Guess parameters

delfe1	=	0.0422810	+/-	0.0123250	(guessed as 0.0
ssfe1	=	0.0050600	+/-	0.0047000	(guessed as 0.0
delfe2	=	-0.1704970	+/-	0.0137850	(guessed as -0.
nfe1a	=	0.5063030	+/-	0.2914520	(guessed as 0.4
nfe1b	=	0.5505380	+/-	0.3310320	(guessed as 0.4
nfe1c	=	0.6513330	+/-	0.3598810	(guessed as 0.5
nfe1d	=	0.4671820	+/-	0.2862200	(guessed as 0.4
nfe2a	=	0.5683350	+/-	0.3168750	(guessed as 0.5
nfe2b	=	0.5138540	+/-	0.3234190	(guessed as 0.4
nfe2c	=	0.4784870	+/-	0.3155270	(guessed as 0.3
nfe2d	=	0.7617610	+/-	0.4179530	(guessed as 0.6

Def parameters (using "FEFFO: Oax at 1.76")

