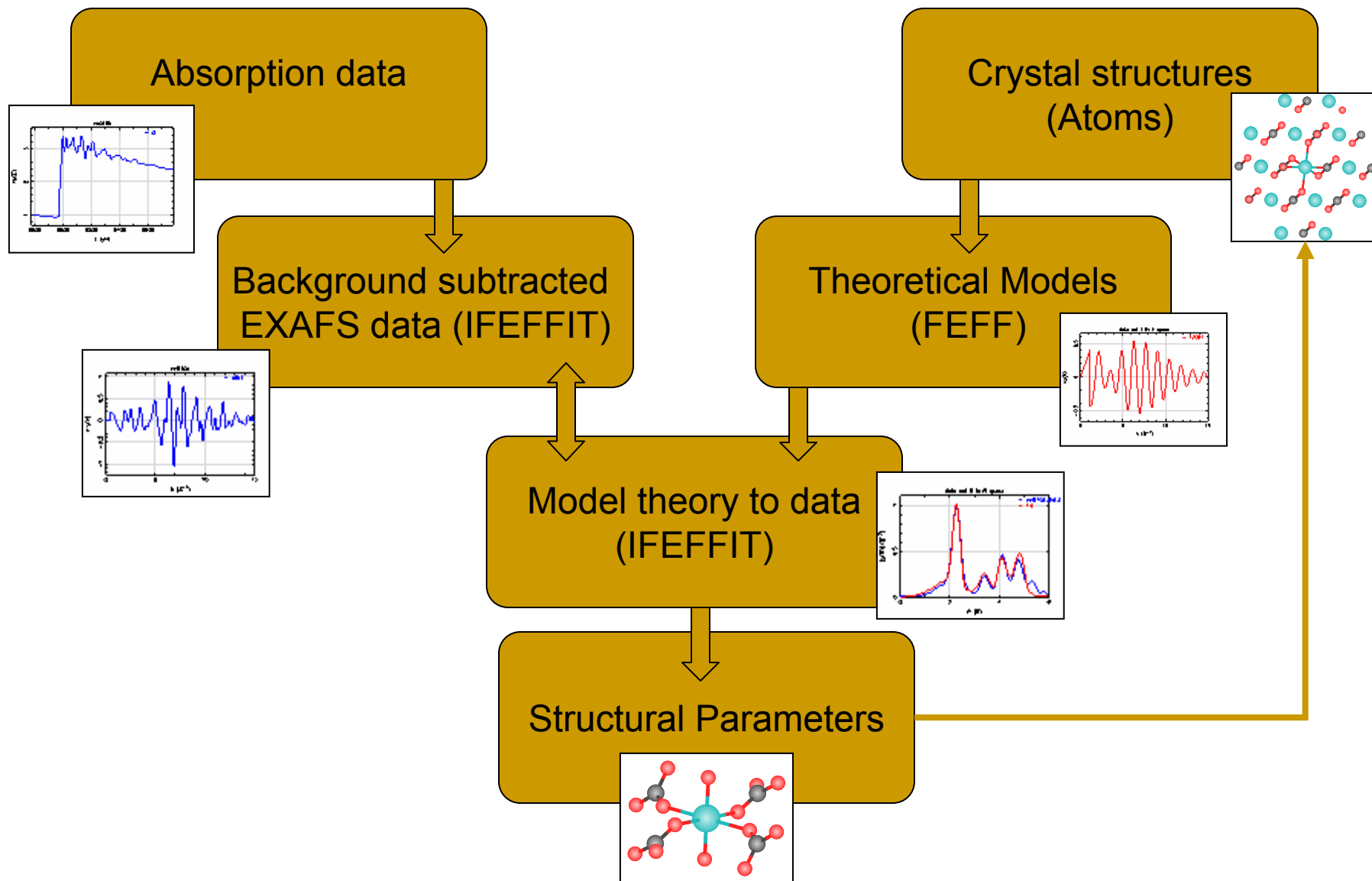

Introduction to EXAFS data analysis

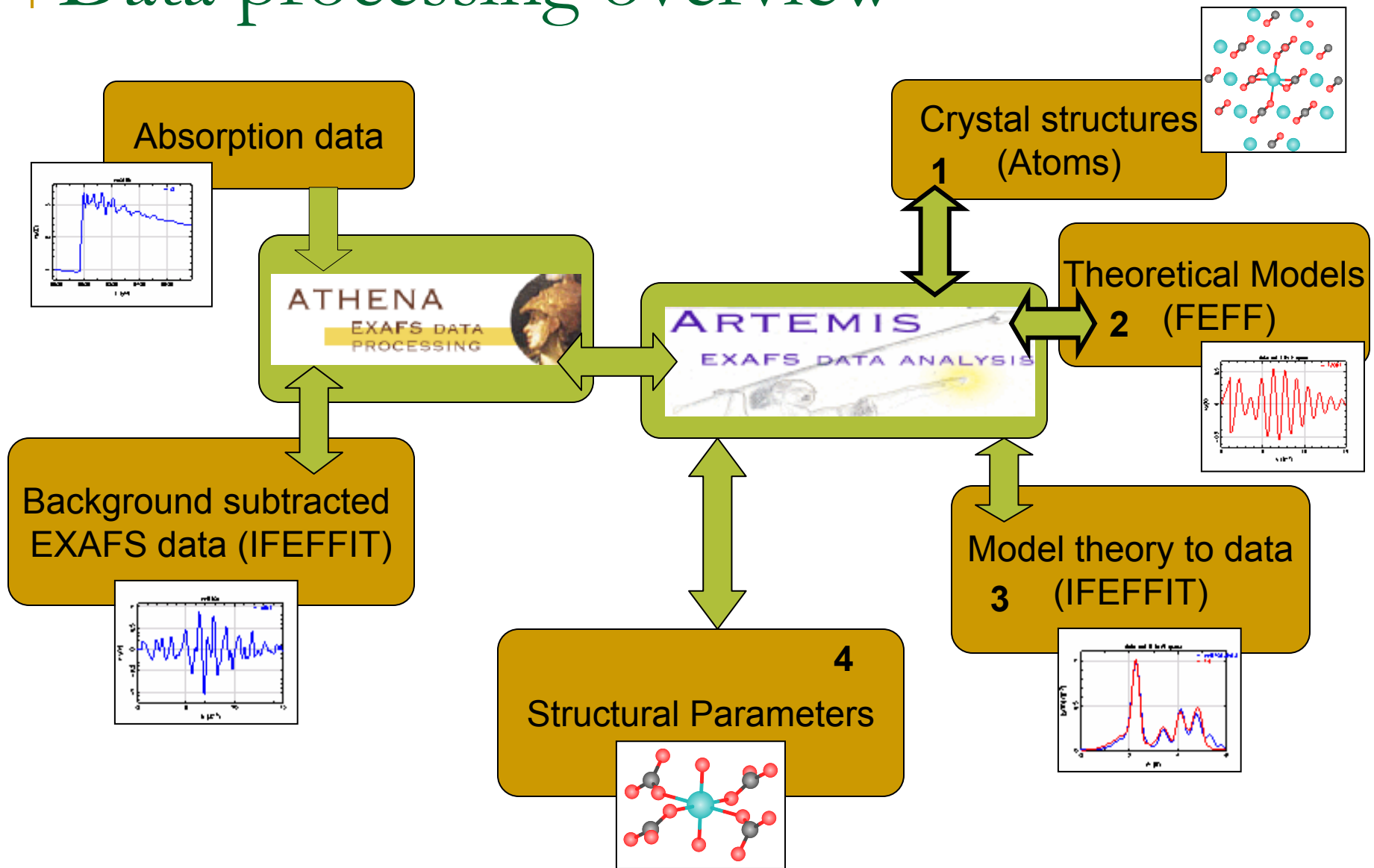
Shelly D. Kelly

Argonne National Laboratory

Data processing overview



Data processing overview



Artemis



Variables

Theory

Project Name:

Data display area:

Changes depending on selected information from Data and Paths list

Echo Area:

Messages from Artemis

The screenshot shows the Artemis software interface. The menu bar includes File, Edit, GDS, Data, FEFF, Paths, Plot, Settings, and Help. The 'Operational Parameters' panel contains fields for Titles, Data file, checkboxes for 'Include data in the fit?', 'Plot data after the fit?', and 'Fit background?'. It also has input fields for k-range, k weight, R-range, k window, R window, Fitting space, Path to use for phase corrections, and Epsilon. The 'Fit' panel on the right shows a 'Data & Paths' list with 'Data' selected. Below it are 'Plot k', 'Plot R', and 'Plot q' buttons, followed by 'Plot k-weight and options' with radio buttons for 0, 1, 2, 3, and kw. At the bottom, there are input fields for kmin, kmax, Rmin, Rmax, qmin, and qmax. A status bar at the bottom left says 'Closing project ... done!'.

Menus:

Fit: optimize variables

Variables

Data: input from Athena

Data and Paths:

Changes data display area

Plotting

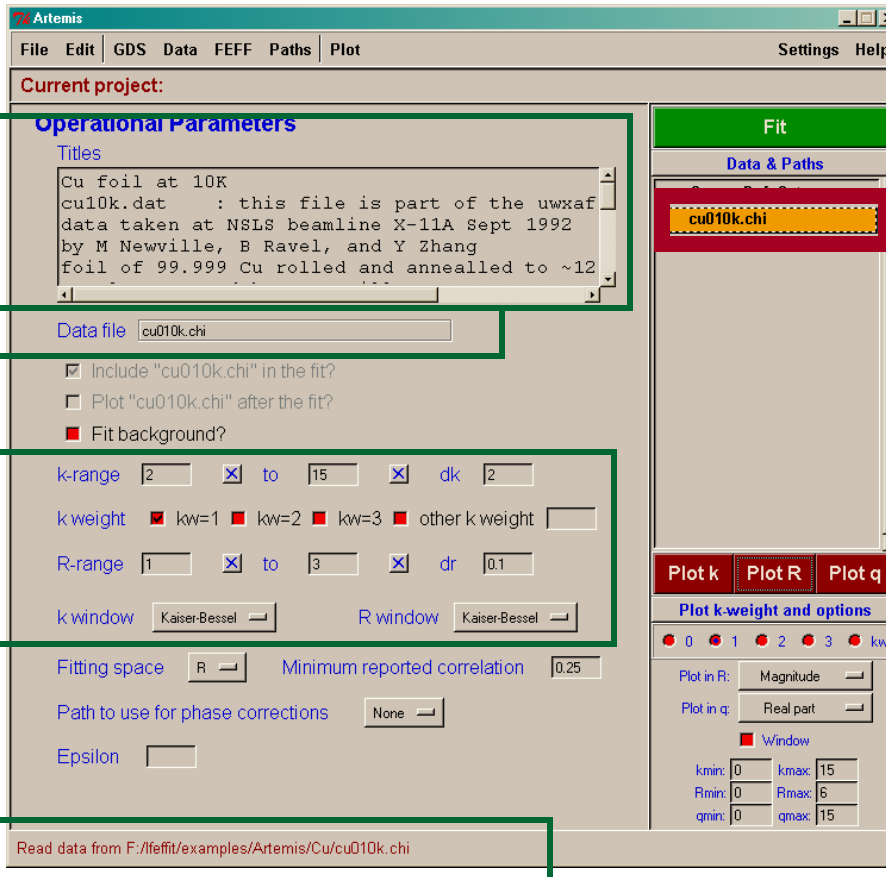
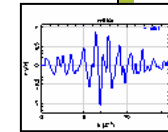
parameters

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

Reading in Data

ATHENA

EXAFS DATA
PROCESSING



The screenshot shows the Artemis software interface. The 'Operational Parameters' panel is highlighted with a green box and contains the following text:

Operational Parameters
Titles
Cu foil at 10K
cu10k.dat : this file is part of the uwxaf
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

Data file: cu010k.chi

Include "cu010k.chi" in the fit?
 Plot "cu010k.chi" after the fit?
 Fit background?

k-range: 2 to 15 dk: 2
k weight: kw=1 kw=2 kw=3 other k weight
R-range: 1 to 3 dr: 0.1
k window: Kaiser-Bessel R window: Kaiser-Bessel

Fitting space: R Minimum reported correlation: 0.25
Path to use for phase corrections: None
Epsilon:

Read data from F:\lfeffit\examples\Artemis\Cu\cu010k.chi

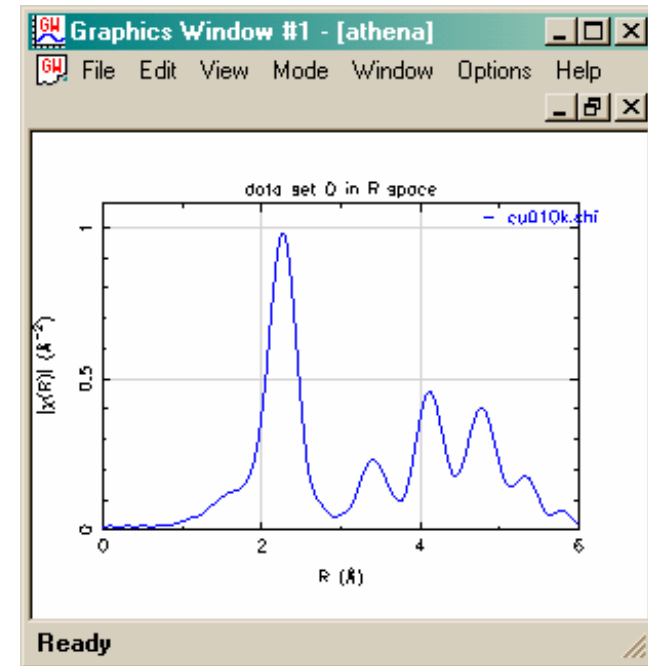
The 'Fit' panel on the right shows 'Data & Paths' with 'cu010k.chi' selected. Below it are buttons for 'Plot k', 'Plot R', and 'Plot q', and a 'Plot k-weight and options' section with radio buttons for '0', '1', '2', '3', and 'kw'. At the bottom, there are input fields for 'kmin', 'kmax', 'Rmin', 'Rmax', 'qmin', and 'qmax'.

Title lines
from data file

data file name

Fourier
transform
parameters

Message from Artemis

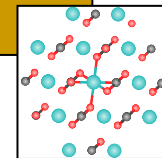


Data plotted in R-space

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

Atoms page

Crystal structures
1 (Atoms)



Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project:
Atoms feff.inp

Titles
Cu 222

Cluster size 7.000 Shift vector 0 0 0
Space group fcc Edge K

A 3.61000 B C
Alpha Beta Gamma

Unique crystallographic sites

Core	El.	X	Y	Z	Tag
1	Cu	0.00000	0.00000	0.00000	
2					
3					
4					
5					
6					
7					
8					
9					
10					
11					

FEFF1

Plot k Plot R Plot q

Plot k-weight and options
0 1 2 3 kw
Plot in R: Magnitude
Plot in q: Real part
Window
kmin: 0 kmax: 15
Rmin: 0 Rmax: 6
qmin: 0 qmax: 15

Run Atoms Add a site

Importing atoms.inp file ... done!

Title lines

Always much larger
than paths used in fit

Structural
Information

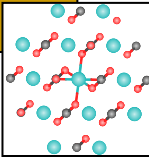
Atom with
a core hole

Make input (feff.inp) for
theoretical calculation
(FEFF)

Message from Artemis

Absorption
edge

➤ Click "Run Atoms"



Theory input page (feff.inp)

Potential list

Atoms list

Atoms generates a list of atoms for Feff, hence the name Atoms.

Run Feff

Current project: feff.inp

POTENTIALS

*	ipot	Z	element
	0	29	Cu
	1	29	Cu

ATOMS

*	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
	0.00000	-1.80500	-1.80500	1	Cu_1
	3.61000	0.00000	0.00000	1	Cu_2
	-3.61000	0.00000	0.00000	1	Cu_2
	0.00000	3.61000	0.00000	1	Cu_2
	0.00000	-3.61000	0.00000	1	Cu_2
	0.00000	0.00000	3.61000	1	Cu_2
	0.00000	0.00000	-3.61000	1	Cu_2
	3.61000	1.80500	1.80500	1	Cu_3
	-3.61000	1.80500	1.80500	1	Cu_3

Run Feff

Importing atoms.inp file ... done!

Fit

Data & Paths

Guess, Def, Set

FEFF1

Plot k Plot R Plot q

Plot k-weight and options

0 1 2 3 kw

Plot in R: Magnitude

Plot in q: Real part

Window

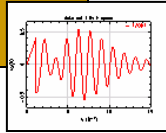
kmin: 0 kmax: 15

Rmin: 0 Rmax: 6

qmin: 0 qmax: 15

➤ Click on Run Feff button

Running Feff



Text messages during Feff calculation

```
Artemis palettes
lfeffit Results Files Messages Echo Journal Properties

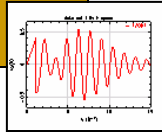
Messages from Artemis
Save buffer to file Dismiss

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
  overlapped potential and density for unique potential
  muffin tin radii and interstitial parameters
  phase shifts for unique potential 0
```

■ 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.

Feff paths: feffxxxx.dat



Current project: feff.inp Interpretation

Interpretation of the FEFF calculation

```
# TITLE Cu 222
#
# Central atom: Copper (29) K edge energy = 8979
# The central atom is denoted by this token: [+]
# Cluster size = 7.0 Angstroms, containing 135 ato
# Curved wave criteria = 2.5.
# Cutoff angle for forward scattering is 20 degree
#
#
```

	degen	reff	amp	fs		scattering path
0001	12	2.553	100.00	:	[+]	Cu_1
0002	6	3.610	22.98	:	[+]	Cu_2
0003	48	3.829	10.59	:	[+]	Cu_1 Cu_1
0004	48	4.358	8.65	:	[+]	Cu_2 Cu_1
0005	24	4.421	55.40	:	[+]	Cu_3
0006	48	4.763	10.62	:	[+]	Cu_1 Cu_1
0007	96	4.763	21.84	:	[+]	Cu_3 Cu_1
0008	12	5.105	18.93	:	[+]	Cu_4
0009	12	5.105	8.46	:	[+]	Cu_1 Cu_1
0010	24	5.105	43.72	1	[+]	Cu_4 Cu_1
0011	12	5.105	8.20	1	[+]	Cu_1
0012	12	5.105	3.56	:	[+]	Cu_1
0014	12	5.105	32.79	2	[+]	Cu_1 Cu_4 Cu_1
0015	48	5.105	3.26	:	[+]	Cu_1 Cu_1 Cu_1
0018	48	5.292	4.14	:	[+]	Cu_3 Cu_1
0019	48	5.292	4.09	:	[+]	Cu_3 Cu_2
0020	96	5.698	2.73	:	[+]	Cu_3 Cu_1
0021	48	5.698	4.80	:	[+]	Cu_3 Cu_3

Legend: Single scattering paths Collinear multiple scattering paths

Fit Data & Paths

Guess, Def, Set

- FEFF2
- feff0001.dat
- feff0002.dat
- feff0003.dat
- feff0004.dat
- feff0005.dat
- feff0006.dat
- feff0007.dat
- feff0008.dat
- feff0009.dat
- feff0010.dat

Plot k Plot R Plot q

Plot k-weight and options

Plot in R: Magnitude

Plot in q: Real part

Window

kmin: 0 kmax: 15

Rmin: 0 Rmax: 6

qmin: 0 qmax: 15

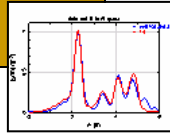
Feff paths

- **Degen:** Degeneracy of the path (number of identical atoms for single scattering path)
- **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.

➤ Click on feff0001.dat in the Data & Paths list

Path Description

Model theory to data
3 (IFEFFIT)

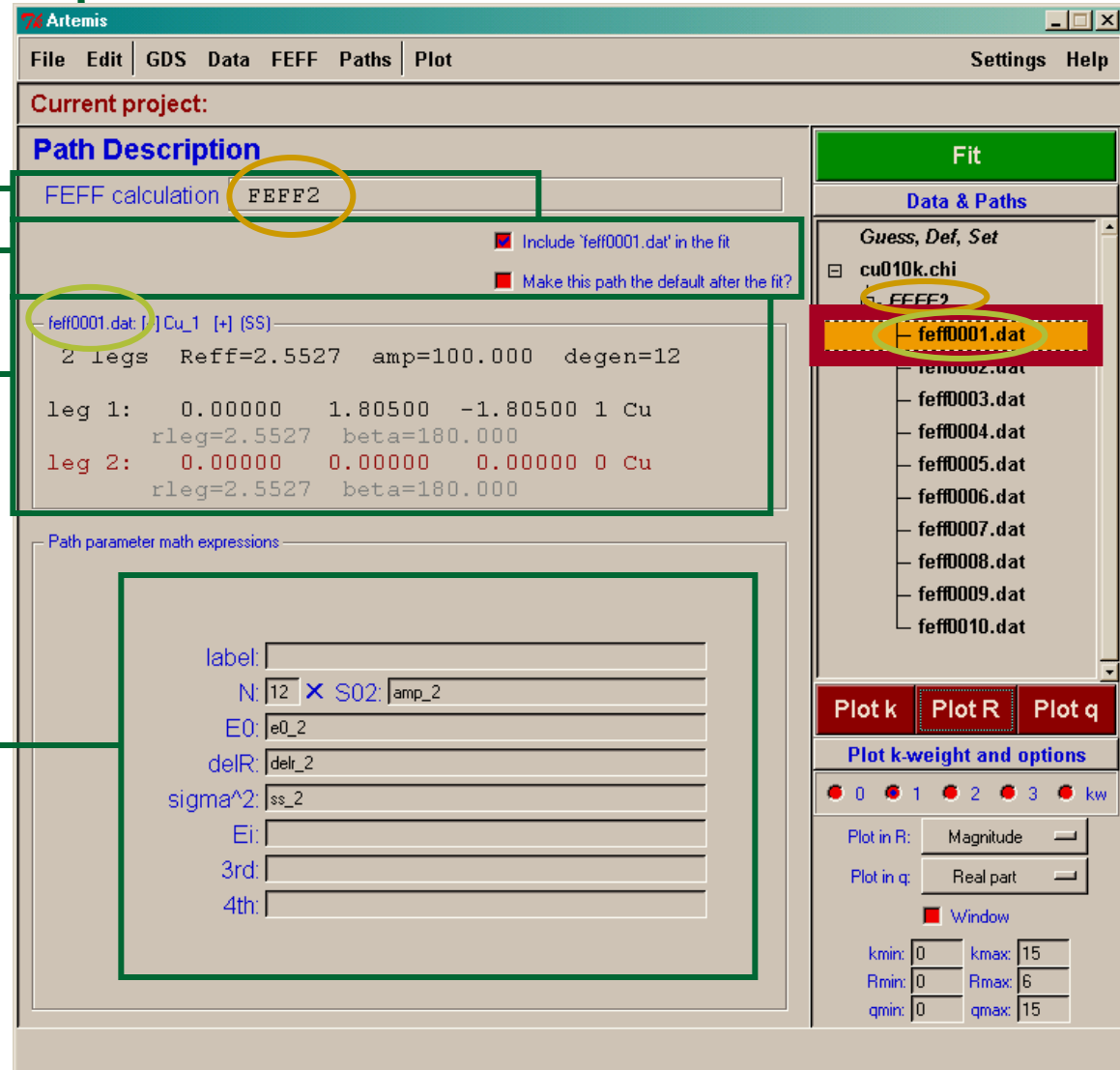


Feff calculation

use or not?

Path description

parameters



The screenshot shows the Artemis software interface with the 'Path Description' window open. The window is divided into several sections:

- Current project:** Path Description
- FEFF calculation:** A dropdown menu showing 'FEFF2' is selected and circled in yellow.
- Include 'feff0001.dat' in the fit:** A checked checkbox.
- Make this path the default after the fit?:** A checked checkbox.
- Path description:** A text area containing:

```
feff0001.dat: [ ] Cu_1 [+](SS)
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:** A text area containing:

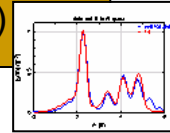
```
label:
N: 12 x S02: amp_2
E0: e0_2
delR: delr_2
sigma^2: ss_2
Ei:
3rd:
4th:
```

On the right side of the interface, the 'Fit' window is open, showing a list of data files. 'feff0001.dat' is highlighted with a red box and a yellow circle. Below the list are buttons for 'Plot k', 'Plot R', and 'Plot q', and a section for 'Plot k-weight and options' with various settings.

The EXAFS Equation

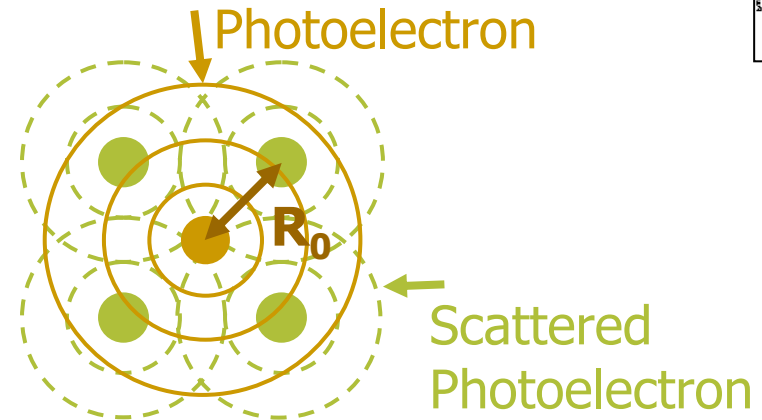
Model theory to data

3 (IFEFFIT)



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

with each path written as:



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

$$R_i = R_0 + \Delta R$$

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

Theoretically calculated values

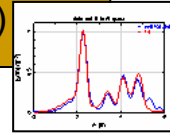
- $F_i(k)$ effective scattering amplitude
- $\phi_i(k)$ effective scattering phase shift
- $\lambda(k)$ mean free path
- R_0 initial path length

Parameters often determined from a fit to data

- N_i degeneracy of path
- S_0^2 passive electron reduction factor
- E_0 energy shift
- ΔR change in half-path length
- σ_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.

The screenshot shows the Artemis software interface. The 'Path Description' section displays the following text:

```
FEFF calculation FEFF2  
 Include 'feff0001.dat' in the fit  
 Make this path the default after the fit?  
  
feff0001.dat: [+] Cu_1 [+] (SS)  
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
```

The 'Path parameter math expressions' section shows the following parameters:

label:	
N:	12 X S02: amp_2
E0:	e0_2
delR:	delr_2
sigma^2:	ss_2
Ei:	
3rd:	
4th:	

The 'Data & Paths' section on the right shows a list of files under 'Guess, Def, Set', with 'feff0001.dat' highlighted in a red box. Below this are buttons for 'Plot k', 'Plot R', and 'Plot q', and a section for 'Plot k-weight and options' with radio buttons for weights 0, 1, 2, 3, and kw.

Parameters often determined from a fit to data

S02 passive electron reduction factor

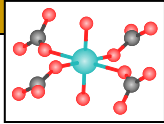
N degeneracy of path

E0 energy shift

delR change in half-path length

sigma^2 mean squared displacement

➤ 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.

#	Name	Math Expression
1	g: amp_2	1
2	d: e0_2	0
3	s: delr_2	0
4	ss_2	0.003
5	r: res1	0.001

Selected parameter: res1 = 0.001

Buttons: Guess Def Set Skip Restrain

Buttons: Define New Grab Discard Hide

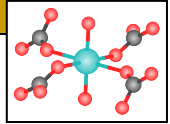
Name of parameters that YOU have created to define the required values for each path

- 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

➤ Click "Fit" to optimize these values

Fit Results

4 Structural Parameters



Artemis palettes

Results from the last fit

Project title : Fitting cu010k.chi
Comment :
Prepared by :
Contact :
Started : 12:18:23 on 9 June, 2004
This fit at : 15:57:04 on 9 June, 2004
Environment : Artemis 0.7.004 using Windows 2000, perl 5.006001, 1

=====
Independent points = 16.18750000
Number of variables = 4.00000000
Chi-square = 958.350319913
Reduced Chi-square = 78.633872403
R-factor = 0.010592234
Measurement uncertainty (k) = 0.001277752
Measurement uncertainty (R) = 0.003818585
Number of data sets = 1.000000000

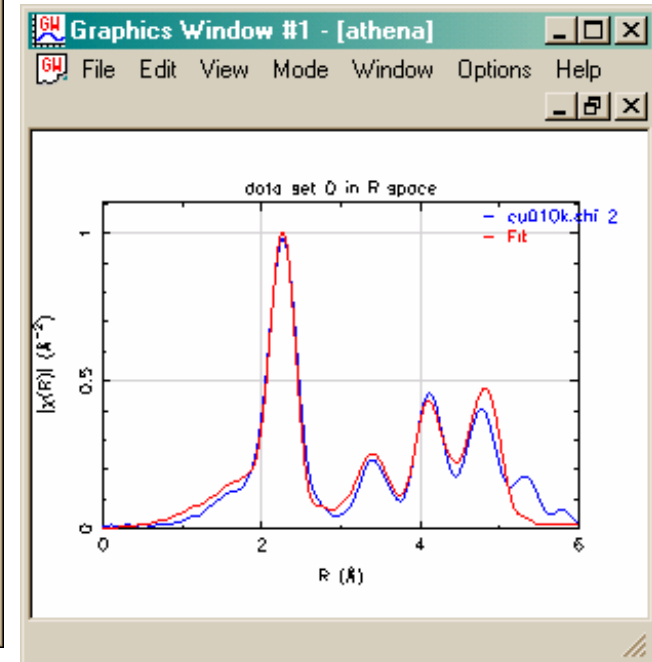
Guess parameters +/- uncertainties:

amp_2	=	0.8622830	+/-	0.0548380	(1.0000)
e0_2	=	4.8386140	+/-	0.5248660	(0.0000)
delr_2	=	-0.0080340	+/-	0.0032900	(0.0000)
ss_2	=	0.0031400	+/-	0.0004780	(0.0030)

Correlations between variables: --> 0.8842
--> 0.7957
All other correlations are below 0.25

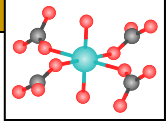
Your parameters

Initial guessed value



➤ Scroll down

Fit Results



```
Artemis palettes
Results Files Messages Echo Journal Properties
Results from the last fit Raw log file Save Dismiss

==== Paths used to fit cu010k.chi 2

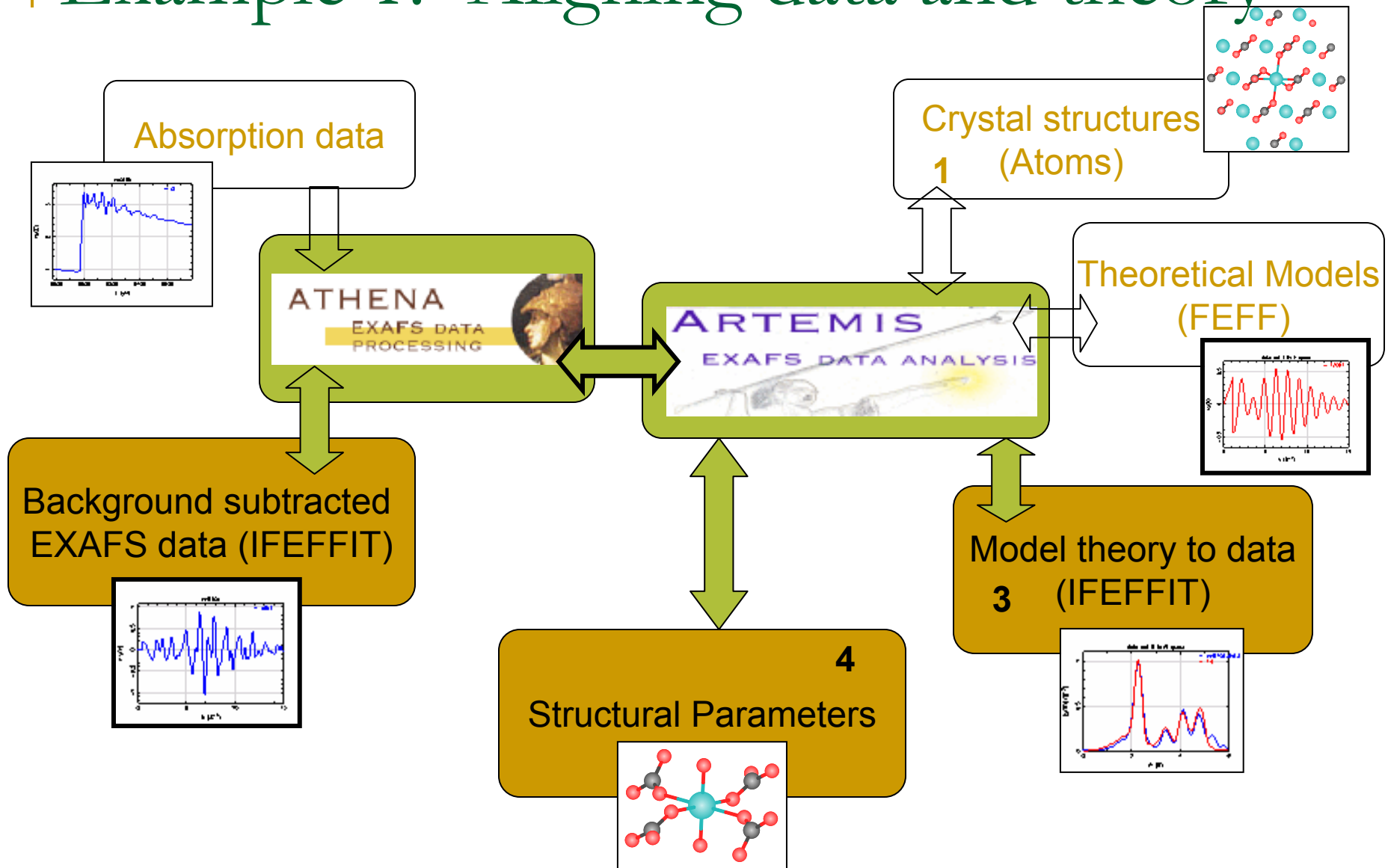
FEFF2: feff0001.dat ..
feff = ENV__IFEFFIT_DIR__\horae\stash\artemis.project.0\data(
id = reff= 2.5527, degen= 12.0, path: Cu->Cu->Cu
r = 2.544666
reff = 2.552700
degen = 12.000000
s02 = 0.862283
e0 = 4.838614
dr = -0.008034
ss2 = 0.003140

FEFF2: feff0002.dat ..
feff = ENV__IFEFFIT_DIR__\horae\stash\artemis.project.0\data(
id = reff= 3.6100, degen= 6.0, path: Cu->Cu->Cu
r = 3.601966
reff = 3.610000
degen = 6.000000
s02 = 0.862283
e0 = 4.838614
dr = -0.008034
ss2 = 0.003140

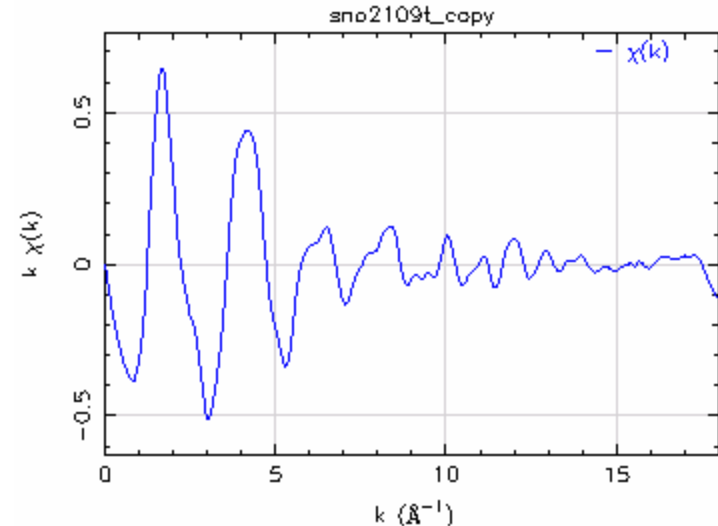
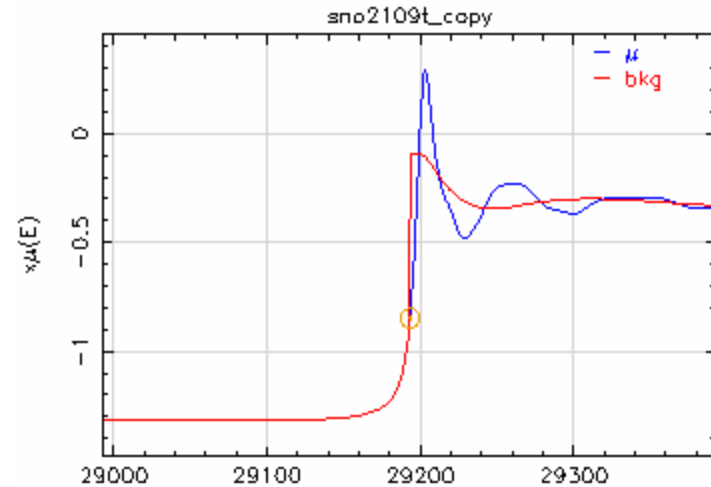
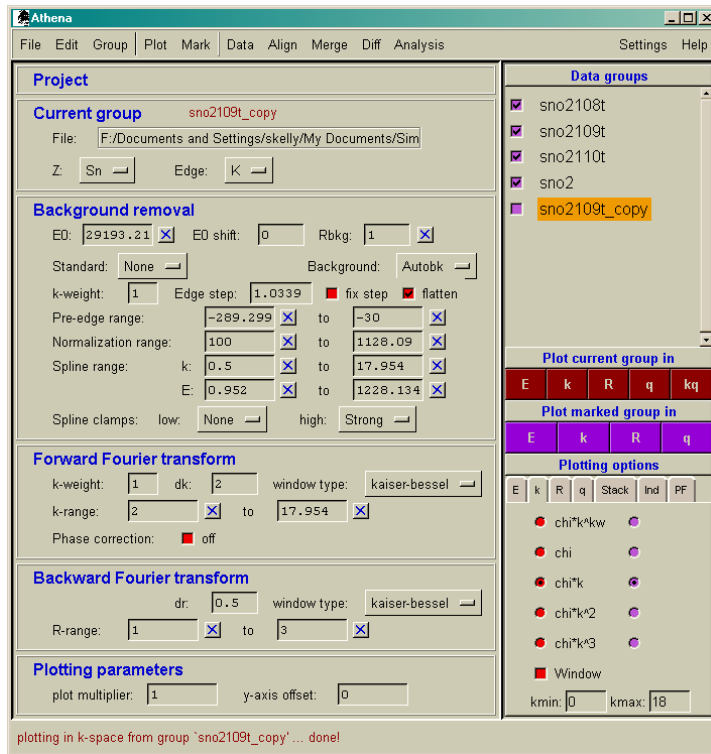
FEFF2: feff0003.dat ..
feff = ENV__IFEFFIT_DIR__\horae\stash\artemis.project.0\data(
id = reff= 3.8290, degen= 48.0, path: Cu->Cu->Cu->Cu
r = 3.820966
reff = 3.829000
degen = 48.000000
s02 = 0.862283
```

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

Example 1: Aligning data and theory



SnO₂ first background removal from Athena



- E0 is somewhere on the edge
- Using default parameters

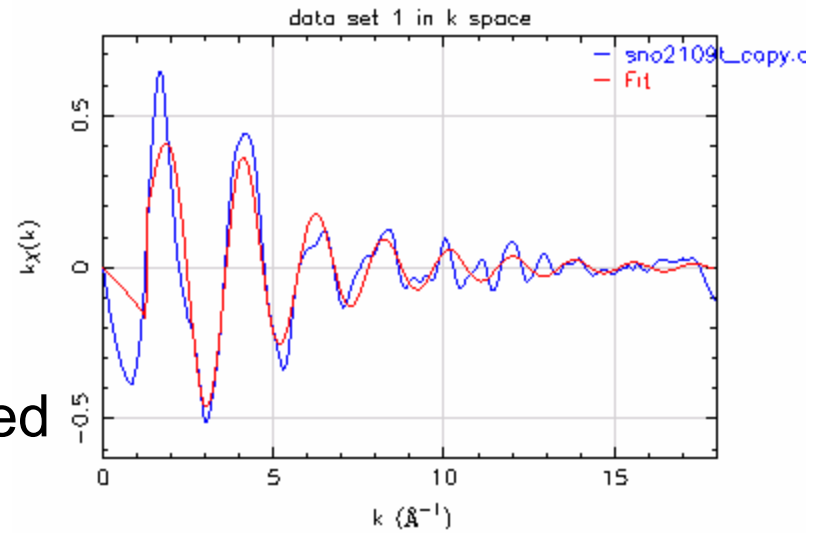
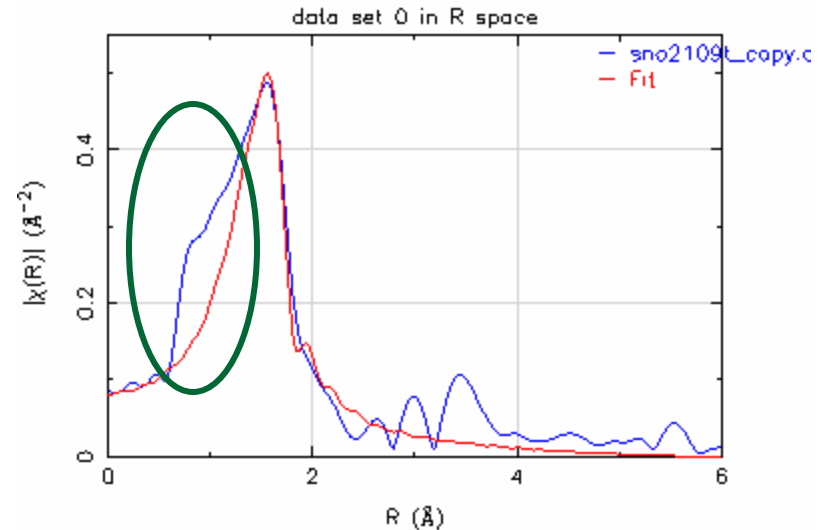
Fit of first Shell

```
Artemis palettes
Results Files Messages Echo Journal Properties
Results from the last fit
Raw log file Save Dismiss
Project title : Fitting sno2109t_copy.chi
Comment :
Prepared by :
Contact :
Started : 10:50:27 on 11 June, 2004
This fit at : 10:54:19 on 11 June, 2004
Environment : Artemis 0.7.004 using Windows 2000, perl 5.006001,

=====
Independent points      =      8.500000000
Number of variables    =      3.000000000
Chi-square             = 48090.666095847
Reduced Chi-square     = 8743.757471972
R-factor               = 0.027192100
Measurement uncertainty (k) = 0.000172798
Measurement uncertainty (R) = 0.000565982
Number of data sets   = 1.000000000

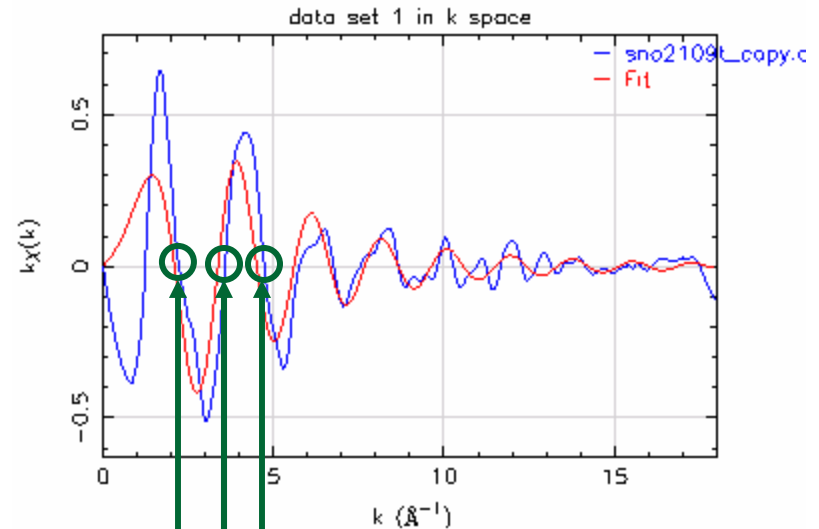
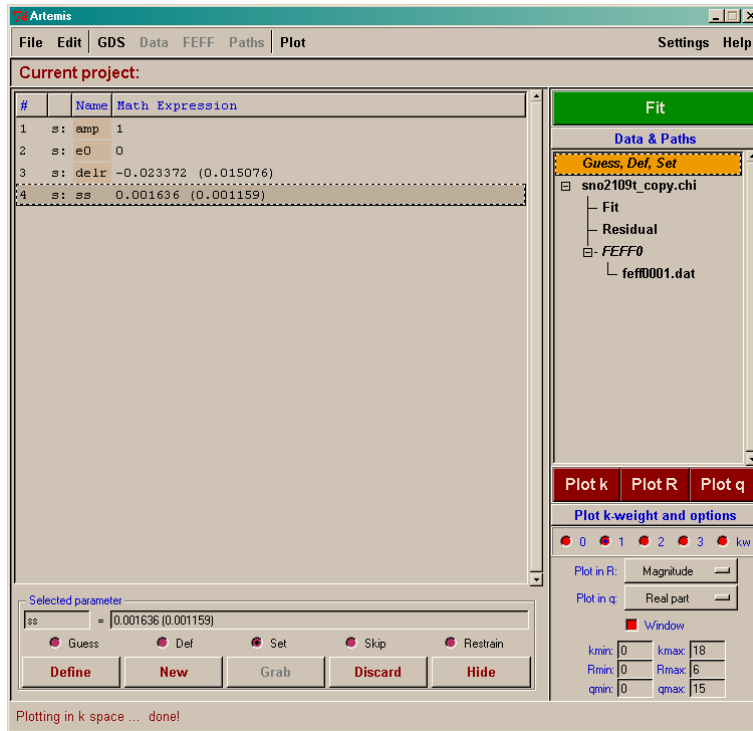
Guess parameters +/- uncertainties:
e0 = 6.2097070 +/- 1.5026480 (0.0000)
delr = -0.0233720 +/- 0.0150760 (0.0000)
ss = 0.0016360 +/- 0.0011590 (0.0030)

Set parameters:
```



- E0 could be smaller
- Background needs to be adjusted

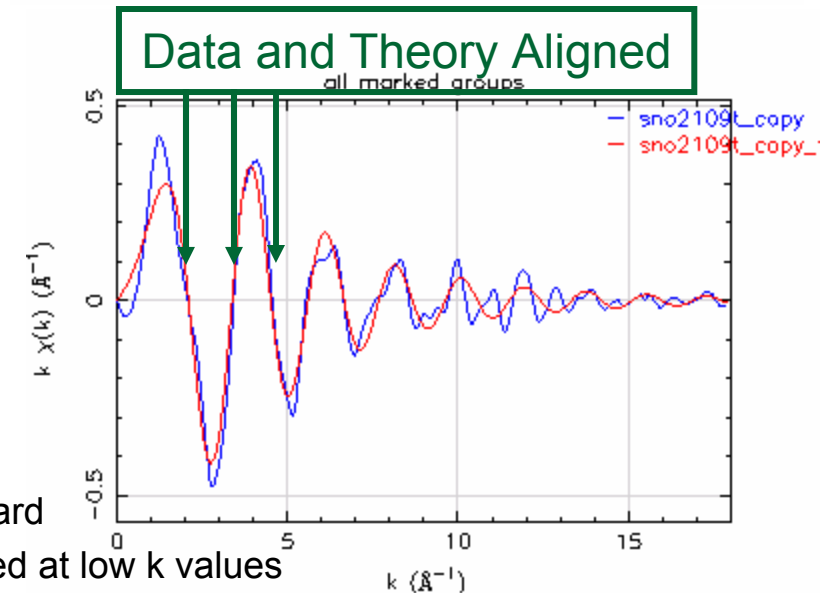
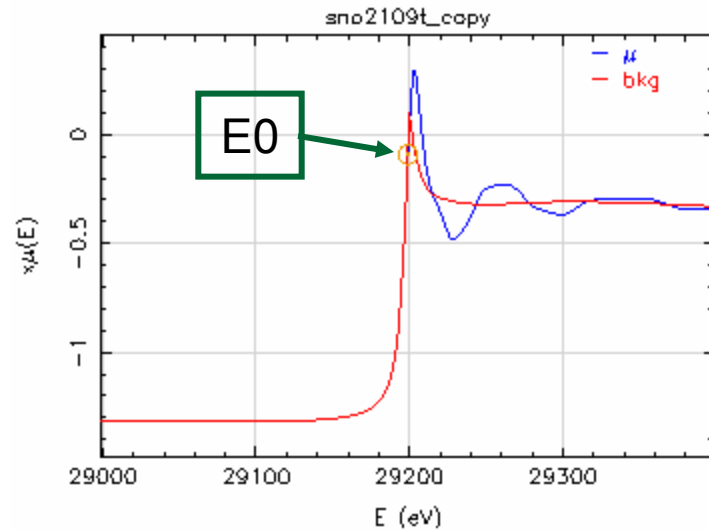
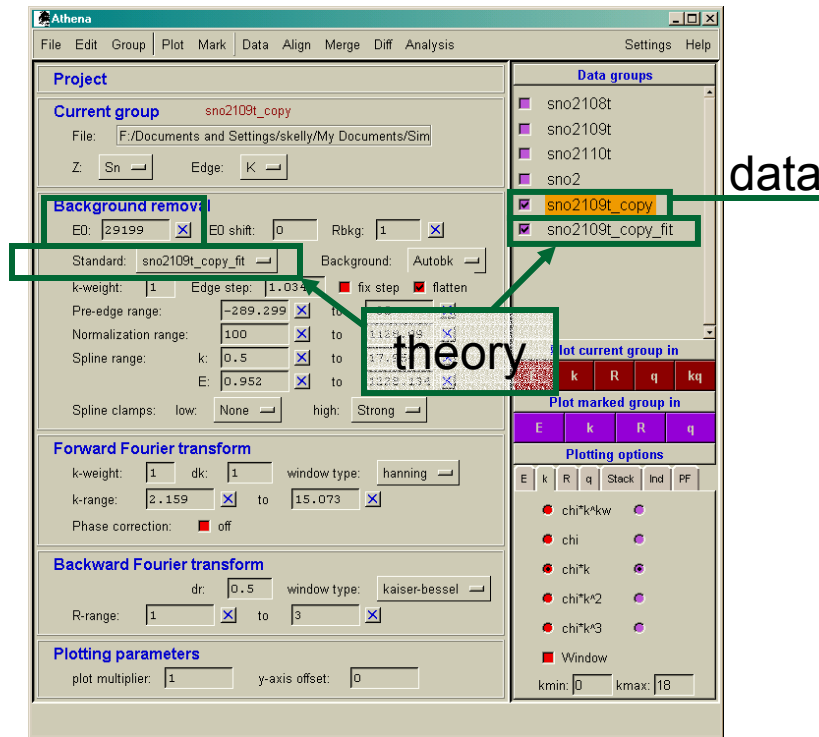
Create first shell model with $E_0=0$



Data and theory are not aligned

- Set parameters to their best-fit values by using the Grab button.
- Change all parameters from guess to set.
- Set $E_0=0$.
- Run the “Fit” again to produce the theory with zero for E_0 .

Background corrected and energy aligned by using theory



- 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

The screenshot shows the Artemis software interface. The main window displays the 'Operational Parameters' and 'Fit' sections. The 'Operational Parameters' section includes titles, data file, and fit options. The 'Fit' section shows the 'Data & Paths' and 'Fit' options. The 'Results from the last fit' section displays the fit statistics and parameters.

Operational Parameters

Titles
Athena data file -- Athena version 0.8.028
Saving sno2109t_copy (group=sno_co?1) as chi(
. Element=Sn Edge=K
Background parameters
E0=29199.000 Eshift=0.000 Rbkg=1.000

Data file: sno2109t_copyth.chi

Include "sno2109t_copyth.chi" in the fit?
 Plot "sno2109t_copyth.chi" after the fit?
 Fit background?

k-range: 2.273 to 15.948 dk: 1
k-weight: kw=1 kw=2 kw=3 other k weight
R-range: 0.373 to 1.970 dr: 0.1
k-window: Hanning R-window: Hanning
Fitting space: R Minimum reported correlation: 0.25
Path to use for phase corrections: None
Epsilon:

Fit

Data & Paths
Guess, Def, Set
sno2109t_copyth.chi
Fit
Residual
FEFF0
feff001.dat

Plot k Plot R Plot q
Plot k-weight and options
Plot in R: Magnitude
Plot in q: Real part
Window
kmin: 0 kmax: 18
Rmin: 0 Rmax: 5
qmin: 0 qmax: 15

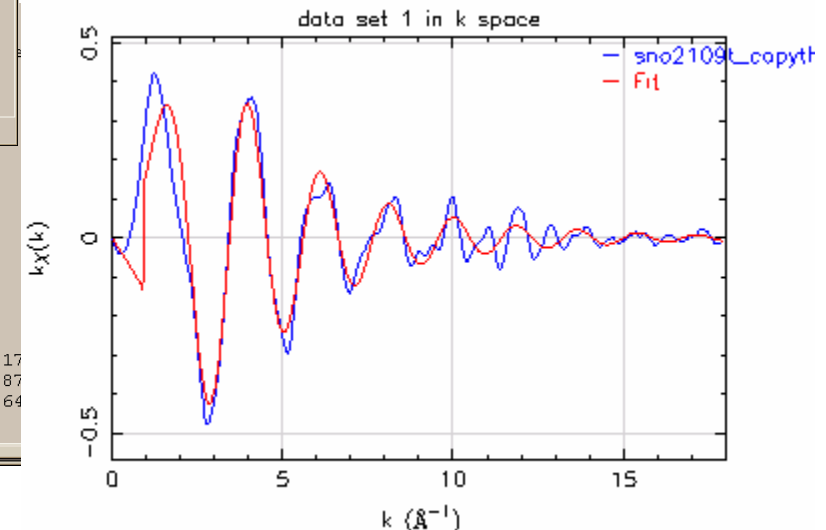
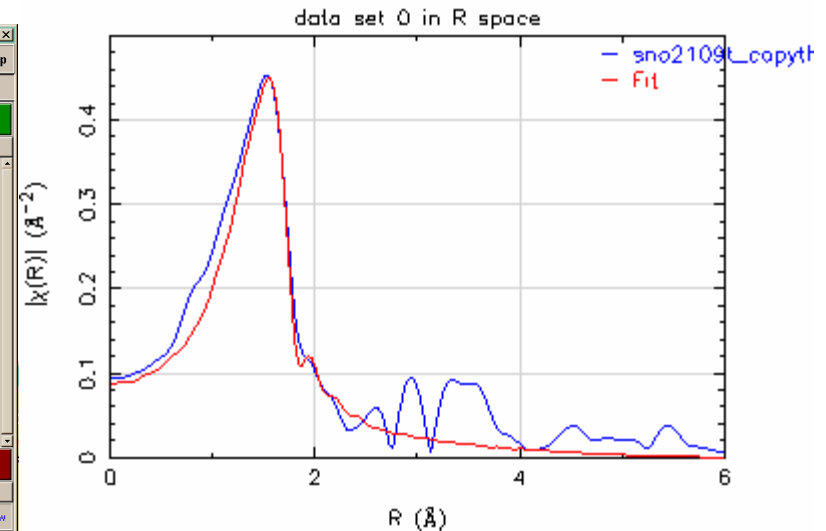
Running fit ... done!

Results from the last fit

Project title : Fitting s
Comment :
Prepared by :
Contact :
Started : 10:50:27
This fit at : 11:03:47
Environment : Artemis 0

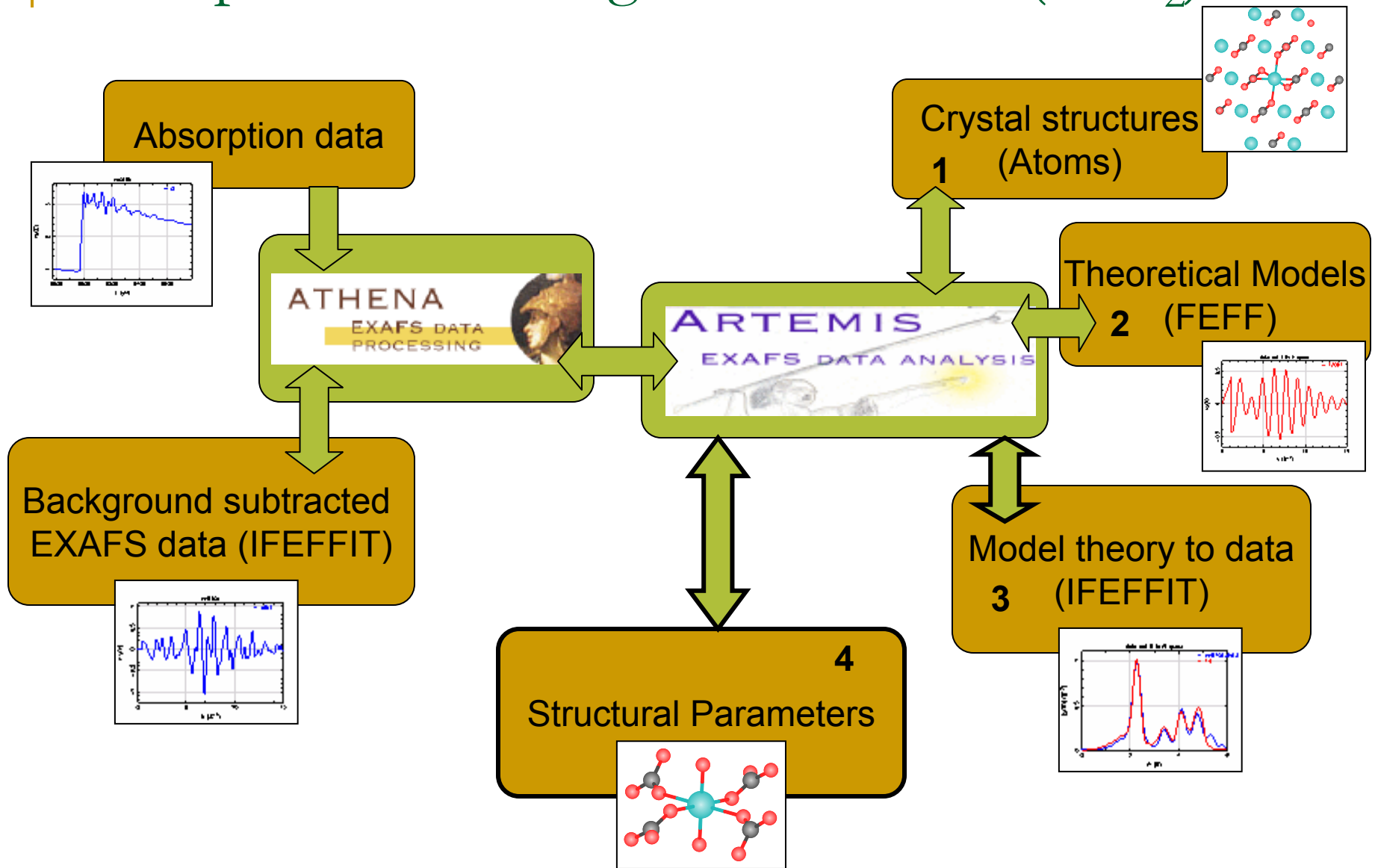
=====
Independent points = 3.00000000
Number of variables = 3.00000000
Chi-square = 13126.463967550
Reduced Chi-square = 2386.629812282
R-factor = 0.008770623
Measurement uncertainty (k) = 0.000168337
Measurement uncertainty (R) = 0.000551370
Number of data sets = 1.00000000

Guess parameters +/- uncertainties:
e0 = 3.1680840 +/- 0.9191780 (guessed as 3.168135 (0.91917
delr = -0.0053310 +/- 0.0087660 (guessed as -0.005331 (0.0087
ss = 0.0020440 +/- 0.0006480 (guessed as 0.002044 (0.00064

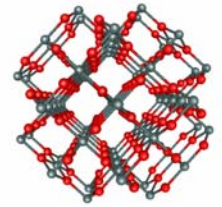


- Read the chi(k) data back into Artemis and fit the first shell

Example 2: Modeling a metal-oxide (SnO_2)



Example 3: Modeling a metal-oxide (SnO_2)



- Compare the sum of all 69 paths to the data

Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project:

#	Name	Math Expression
1	amp	1
2	e0	0
3	delr	0
4	as	0.003

Fit

Data & Paths

Guess, Def, Set

- chi.chi
- Fit
- Residual
- FEFF0
 - feff0001.dat
 - feff0002.dat
 - feff0003.dat
 - feff0004.dat
 - feff0005.dat
 - feff0006.dat
 - feff0007.dat
 - feff0008.dat
 - feff0009.dat

Plot k Plot R Plot q

Plot kweight and options

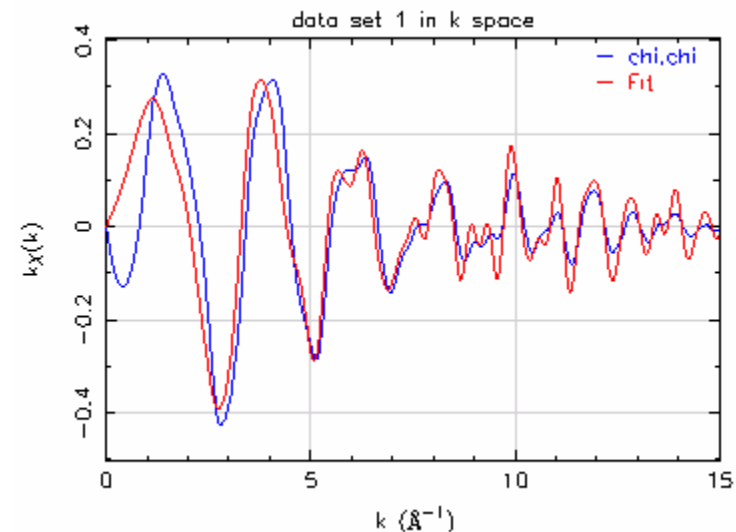
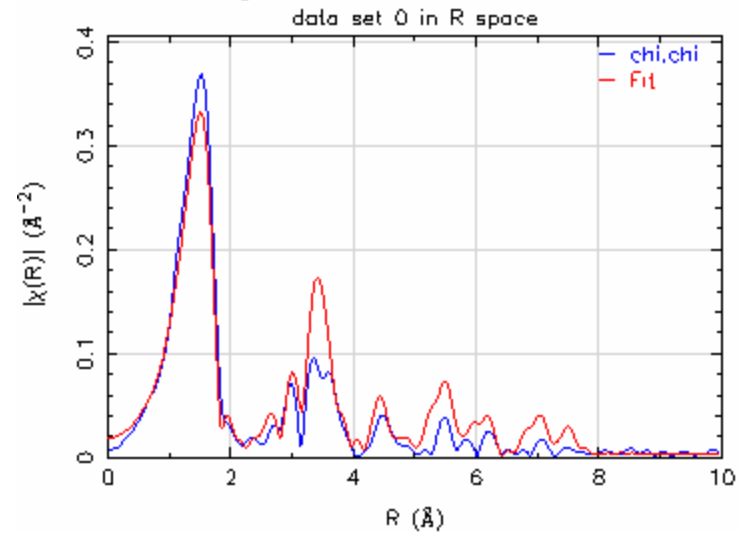
Plot in R: Magnitude

Plot in q: Real part

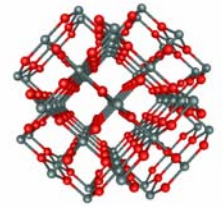
Window

kmin	0	kmax	15
Rmin	0	Rmax	10
qmin	0	qmax	15

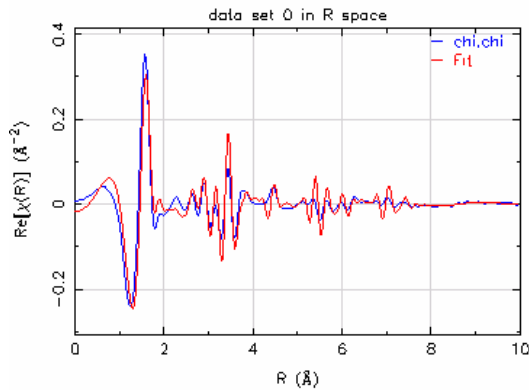
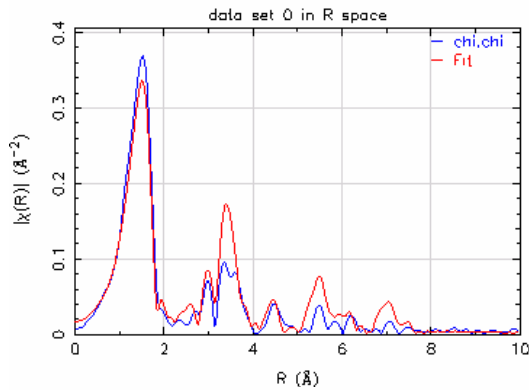
Plotting in k space done!



How many paths are required?

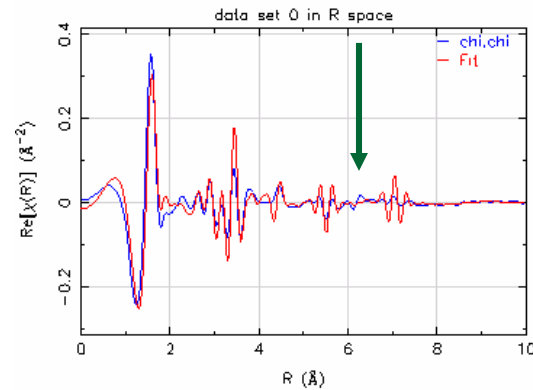
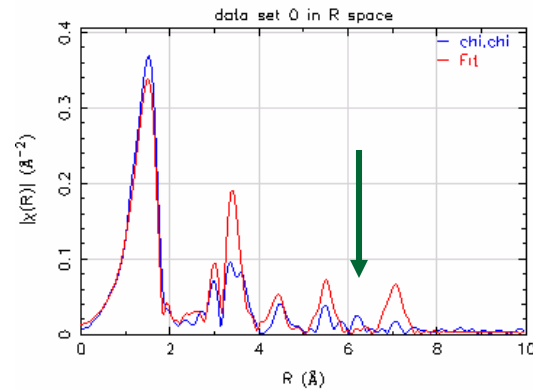


Minimum amplitude 5%
30 of 69 paths



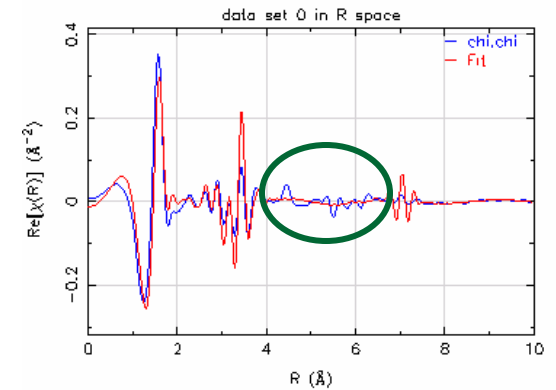
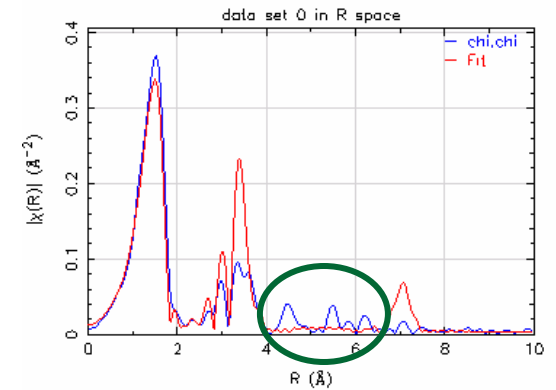
All data is present in model

Minimum amplitude 10%
18 of 69 paths



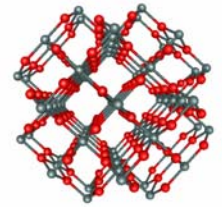
missing a little of the data

Minimum amplitude 15%
8 of 69 paths



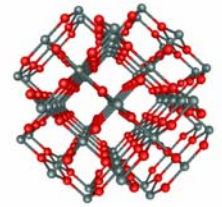
missing a lot of the data

Models to consider:



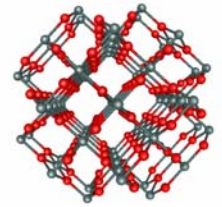
- Δr :
 - Symmetric expansion term: $\text{Alpha} * \text{reff}$.
 - Grouped depending on distance and atom types
 - Related to unit cell dimensions
- ΔE :
 - Energy shifts that depend on atom type
 - One energy shift for all paths
 - Two energy shifts, one for first shell and another for all other shells
- σ^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 where N is expected to change.

The Model for SnO₂ data

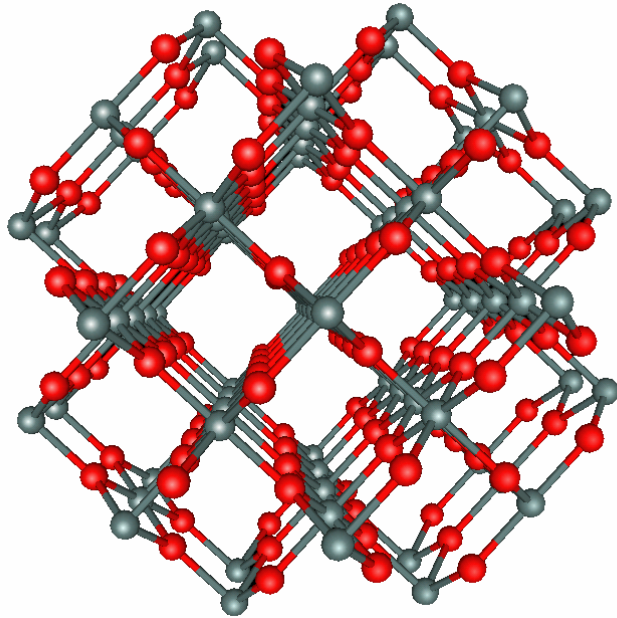


- Δr : symmetric expansion term: $\text{Alpha} * \text{reff}$.
- ΔE : Energy shifts that depend on atom type:
 - The first shell; E_{o1} ,
 - All other oxygen scattering events: E_{o2}
 - All tin scattering events: E_{sn}
- σ^2 : Grouped depending on distance and atom types.
- S_{02} : one for all paths.
- N : determined from the crystal structure.

Final Model for SnO₂



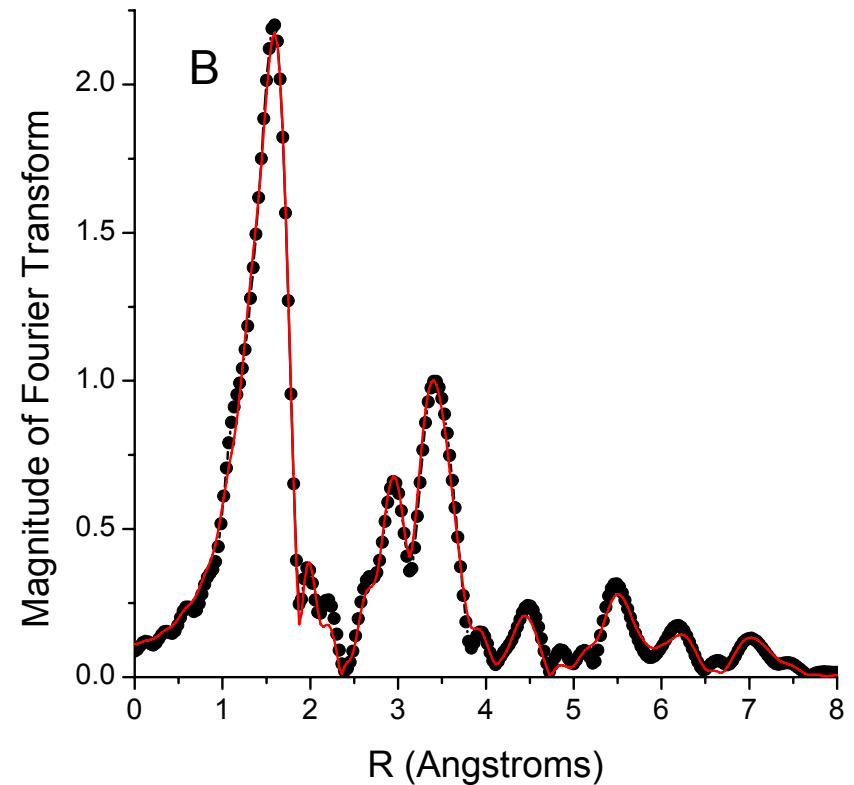
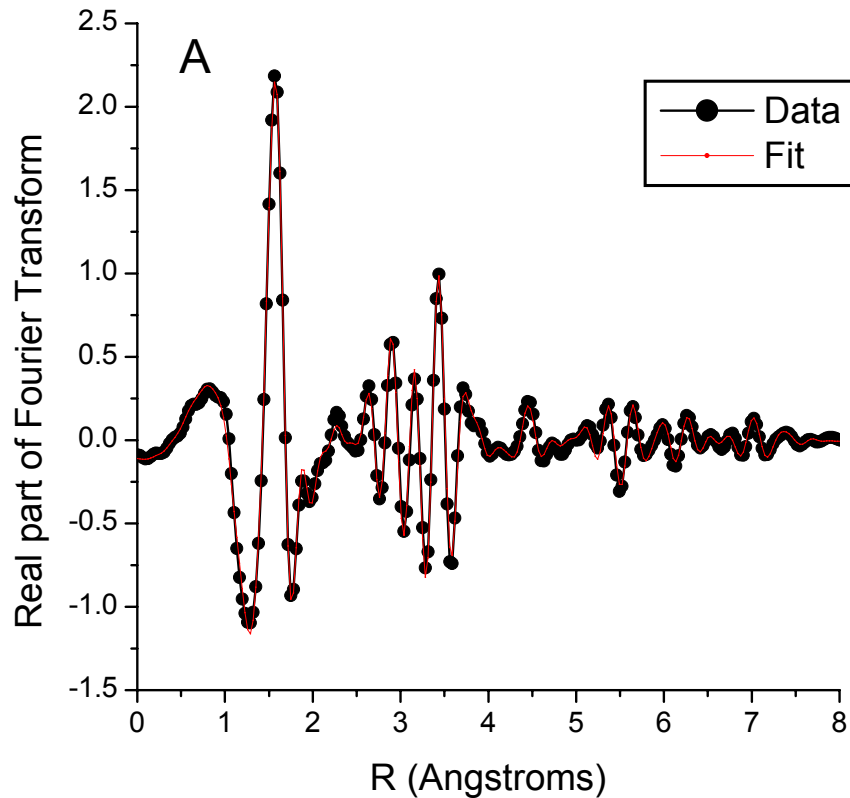
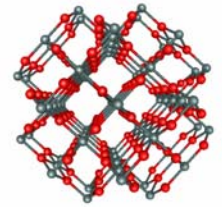
Includes all the atoms shown here



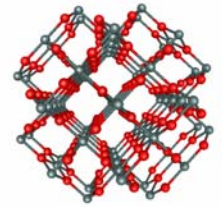
<i>Path</i>	<i>N</i>	<i>reff</i>	ΔR	σ^2	ΔE
Sn-O1	4	2.0519	Alpha-reff	σ^2_{o1}	ΔE_{o1}
Sn-O2	2	2.0567	Alpha-reff	σ^2_{o1}	ΔE_{o1}
Sn-Sn1	2	3.1864	Alpha-reff	σ^2_{sn1}	ΔE_{sn}
Sn-O3	4	3.5906	Alpha-reff	σ^2_{o3}	ΔE_{o2}
Sn-Sn2	8	3.7093	Alpha-reff	σ^2_{sn2}	ΔE_{sn}
Sn-Sn2-O1	8	3.9090	Alpha-reff	σ^2_{sn2o1}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn2-O2	8	3.9090	Alpha-reff	σ^2_{sn2o1}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-O5	8	4.2414	Alpha-reff	σ^2_{o5}	ΔE_{o2}
Sn-Sn3	4	4.7373	Alpha-reff	σ^2_{sn3}	ΔE_{sn}
Sn-O7	8	4.8006	Alpha-reff	σ^2_{o7}	ΔE_{o2}
Sn-Sn4	8	5.7092	Alpha-reff	σ^2_{sn4}	ΔE_{sn}
Sn-Sn5	8	5.8365	Alpha-reff	σ^2_{sn4}	ΔE_{sn}
Sn-Sn5-O1	8	5.8405	Alpha-reff	σ^2_{sn4}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn5-O4	8	5.8405	Alpha-reff	σ^2_{sn4}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o2}$
Sn-O1-Sn5-O1	4	5.8444	Alpha-reff	σ^2_{sn4}	$0.33 \cdot \Delta E_{sn} + 0.66 \cdot \Delta E_{o1}$
Sn-O4-Sn5-O4	4	5.8444	Alpha-reff	σ^2_{sn4}	$0.33 \cdot \Delta E_{sn} + 0.66 \cdot \Delta E_{o2}$
Sn-Sn6-Sn1	4	6.3728	Alpha-reff	σ^2_{sn6}	ΔE_{sn}
Sn-Sn1-Sn6-Sn1	2	6.3728	Alpha-reff	σ^2_{sn6}	ΔE_{sn}
Sn-Sn7	4	6.6995	Alpha-reff	σ^2_{sn7}	ΔE_{sn}
Sn-Sn7-O2	4	6.6995	Alpha-reff	σ^2_{sn7}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o1}$
Sn-Sn7-O6	4	6.6995	Alpha-reff	σ^2_{sn7}	$0.5 \cdot \Delta E_{sn} + 0.5 \cdot \Delta E_{o2}$
Sn-Sn7-O6-O2	4	6.6995	Alpha-reff	σ^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-reff	σ^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-reff	σ^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-reff	σ^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-reff	σ^2_{sn8}	ΔE_{sn}
Sn-Sn8-Sn2	16	7.4187	Alpha-reff	σ^2_{sn8}	ΔE_{sn}
Sn-Sn2-Sn8-Sn2	8	7.4187	Alpha-reff	$4 \cdot \sigma^2_{sn8}$	ΔE_{sn}
Sn-Sn2-Sn8-Sn2	8	7.4187	Alpha-reff	σ^2_{sn8}	ΔE_{sn}
Sn-Sn9	16	7.6578	Alpha-reff	σ^2_{sn9}	ΔE_{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_2



Evaluating fit Results



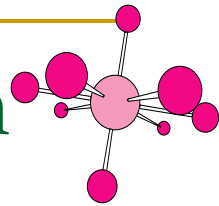
Typical values for EXAFS parameters

- Δr : less than 0.5 Å
- ΔE : less than 10 eV
- σ^2 : 0.003 to 0.020 Å²
- $S02$: 0.70 to 1.10

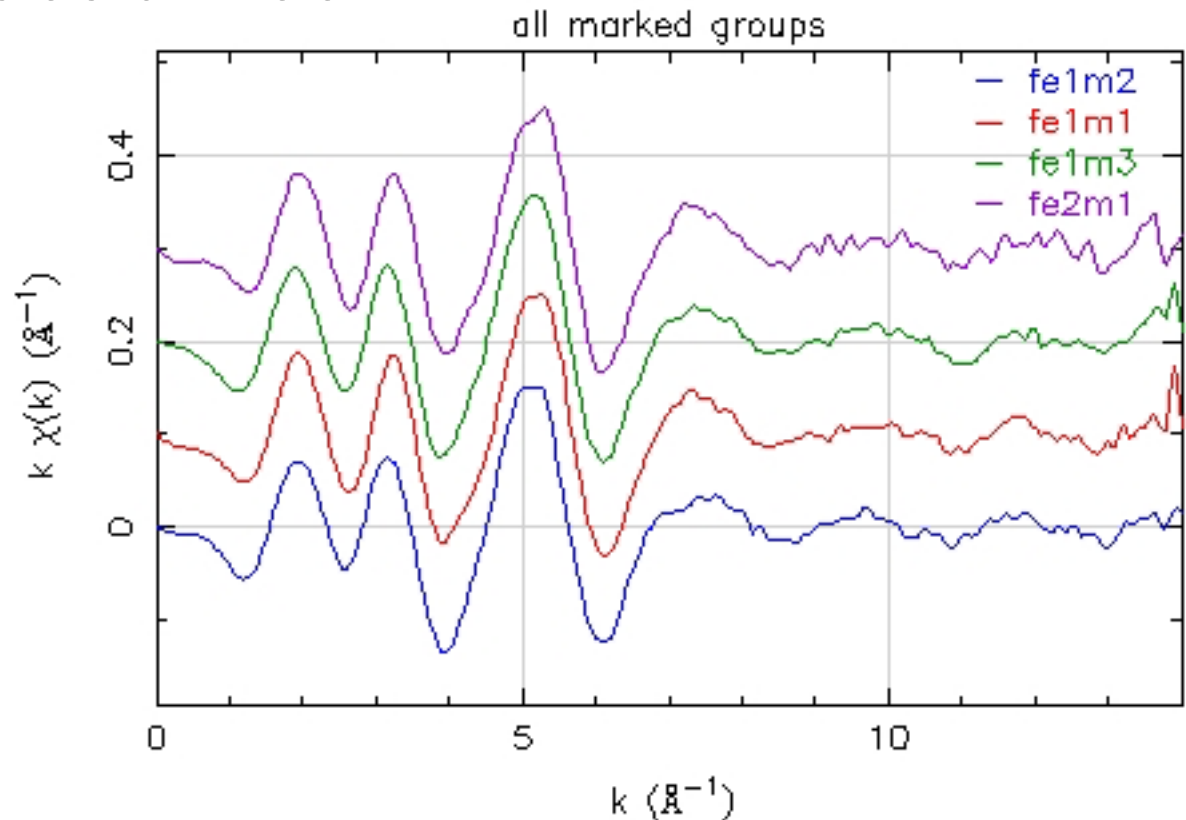
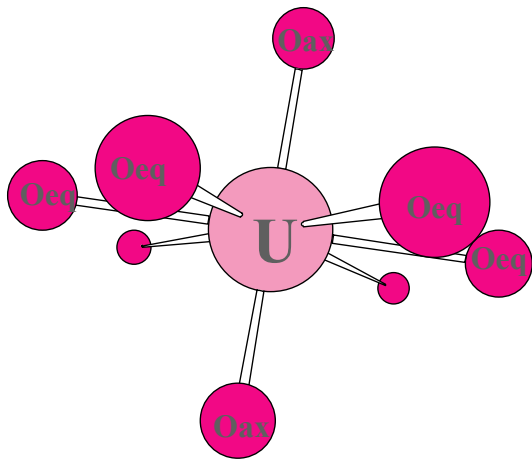
```
Artemis palettes
feffit Results Files Messages Echo Journal Properties
Results from the last fit Raw log file Save Dismiss
Project title : Fitting chi.chi
Comment      :
Prepared by  : skelly@little.er.anl.gov
Contact      :
Started      : 09:28:09 on 11 May, 2004
This fit at  : 14:34:33 on 11 June, 2004
Environment  : Artemis 0.7.004 using Windows 2000, perl 5.006001, Tk 8.5.3
=====
Independent points      =      56.581054688
Number of variables    =      18.000000000
Chi-square             =     17173.011916455
Reduced Chi-square     =     445.115149276
R-factor              =      0.009620226
Measurement uncertainty (k) =    0.000131921
Measurement uncertainty (R) =    0.000425961
Number of data sets    =      1.000000000

Guess parameters +/- uncertainties:
amp      =    1.0730830 +/-    0.0234380 (1.0731)
eo1      =    3.4103970 +/-    0.2153030 (3.4017)
esn      =    2.7078640 +/-    0.5056810 (2.6664)
eo2      =    5.0721730 +/-    0.8724980 (5.0268)
alpha    =   -0.0000610 +/-    0.0007560 (-0.0001)
sso1     =    0.0034200 +/-    0.0002940 (0.0034)
sso2     =    0.0203500 +/-    0.0071200 (0.0203)
sso4     =    0.0066190 +/-    0.0022170 (0.0066)
sso6     =    0.0066140 +/-    0.0036570 (0.0066)
sssn2o1  =    0.0039560 +/-    0.0012540 (0.0040)
sssn1    =    0.0037940 +/-    0.0003000 (0.0038)
sssn2    =    0.0054140 +/-    0.0002360 (0.0054)
sssn3    =    0.0070590 +/-    0.0013390 (0.0071)
sssn4    =    0.0076870 +/-    0.0006680 (0.0077)
sssn5    =    0.0089770 +/-    0.0029180 (0.0090)
sssn6    =    0.0065650 +/-    0.0022060 (0.0066)
sssn7    =    0.0089890 +/-    0.0016540 (0.0086)
sssn8    =    0.0107550 +/-    0.0041580 (0.0096)
```

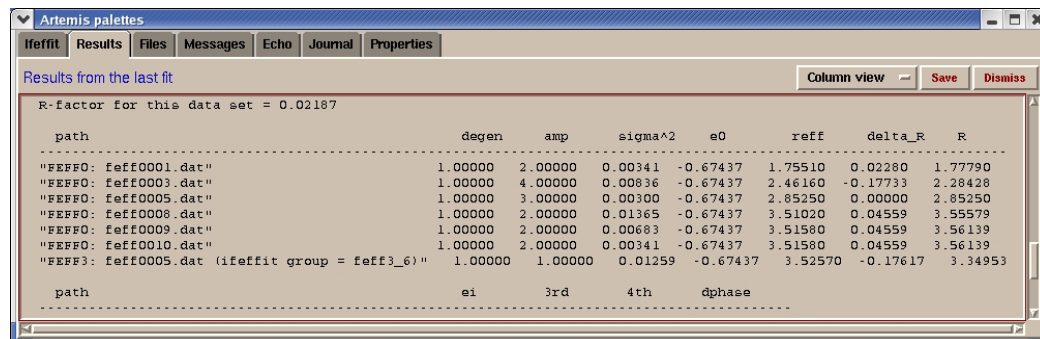
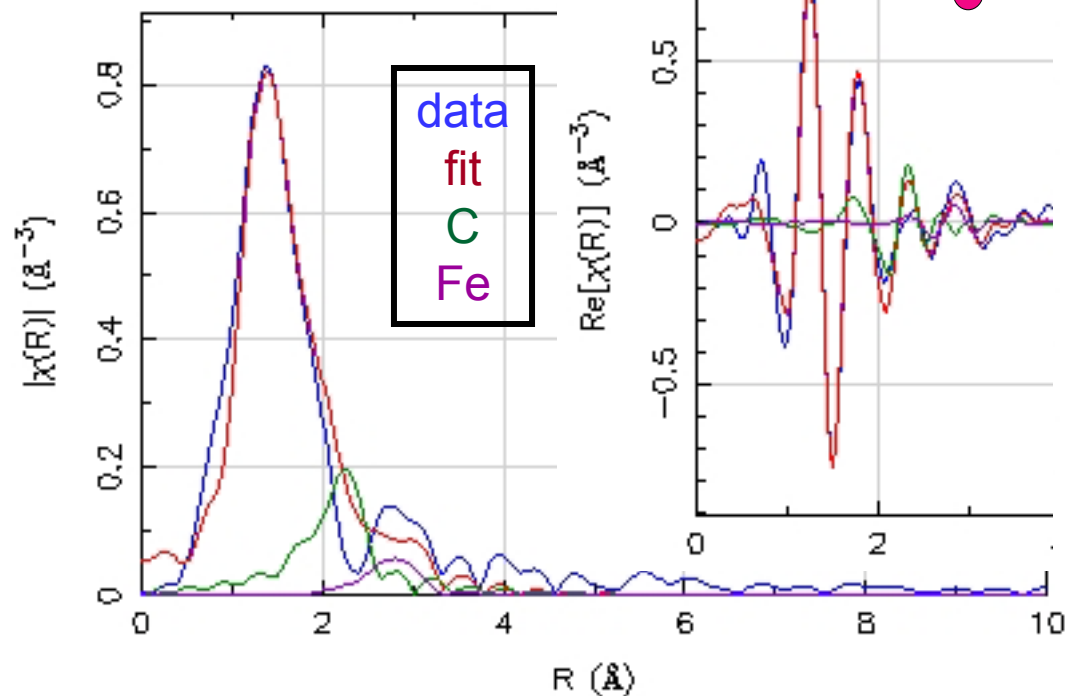
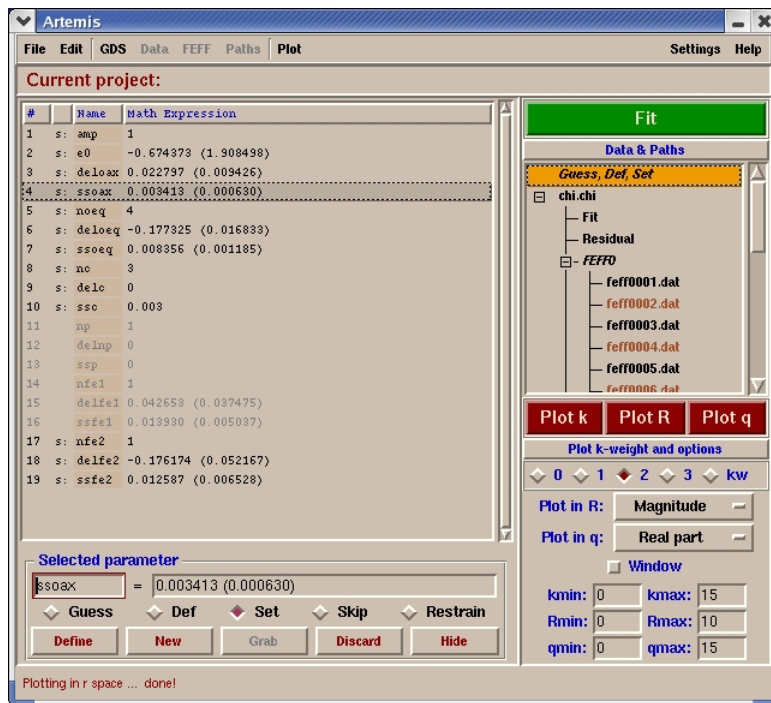
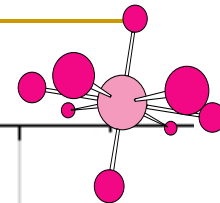
Example 3: Determining 2nd shell atom type and number



- 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

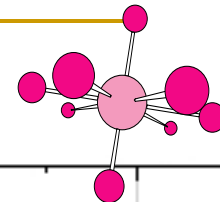


Test data for C and Fe shells

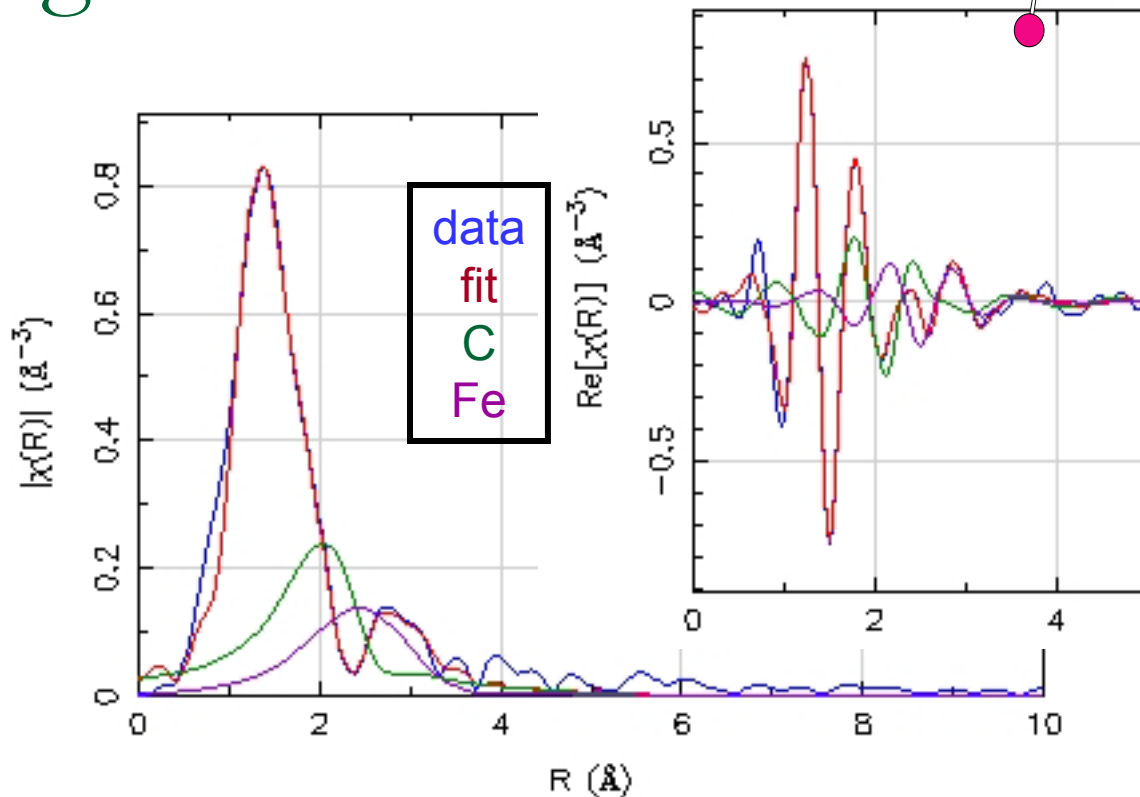


- Place **C** and **Fe** shells in a "good" spot
 - set parameters – no fitting
 - monitor results and fit spectra

Fit Results using C and Fe shells



EXAFS Parameters	
σ^2 -values	-
Distances	+
Coordination numbers	-
ΔE -value	-



Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

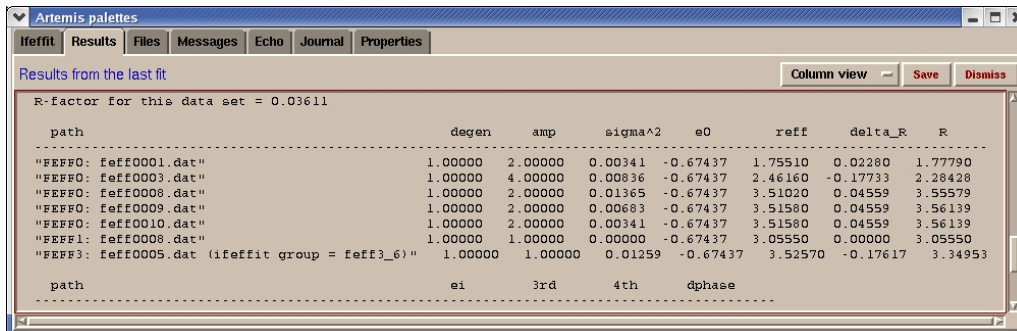
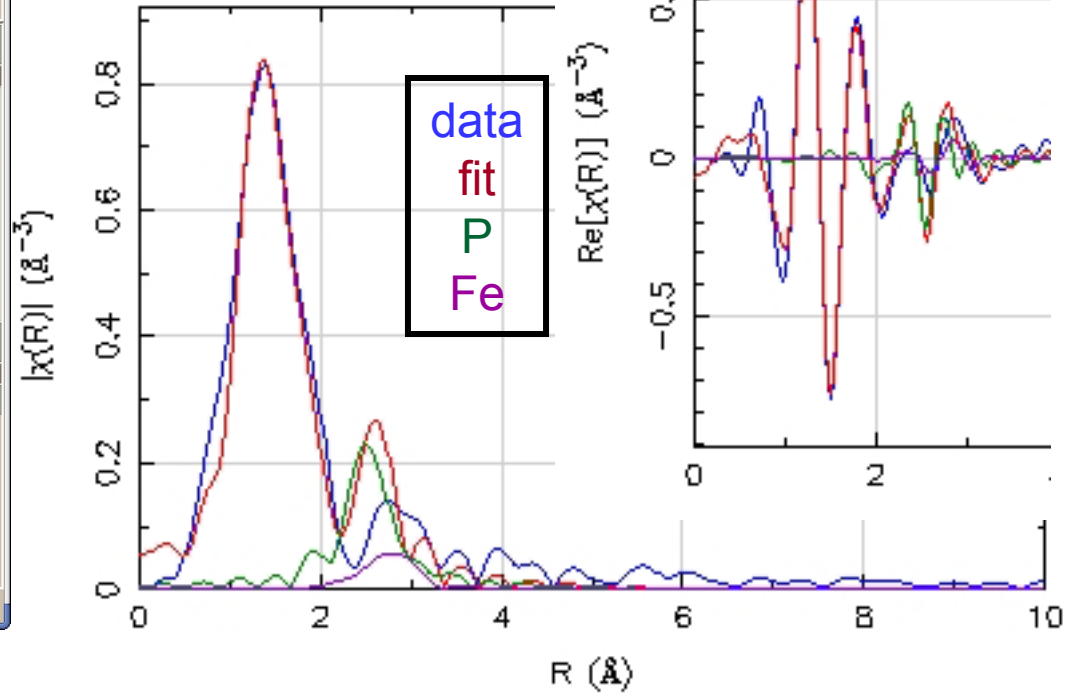
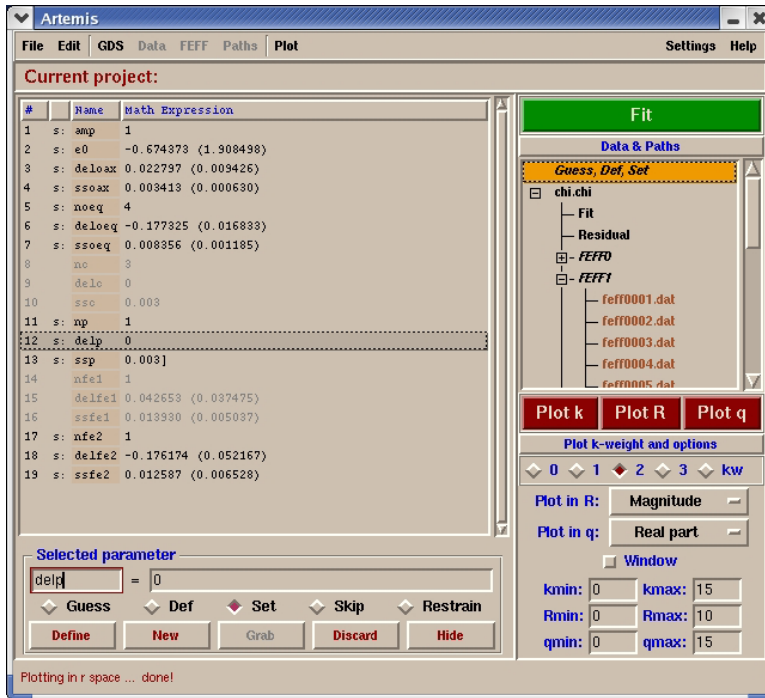
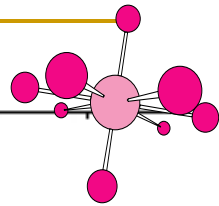
Results from the last fit Column view Save Dismiss

R-factor for this data set = 0.00168

path	degen	amp	sigma^2	e0	reff	delta_R	R
"FEFF0: feff0001.dat"	1.00000	2.00000	0.00367	-8.43947	1.75510	-0.00547	1.74963
"FEFF0: feff0003.dat"	1.00000	4.72819	0.00935	-8.43947	2.46160	-0.22032	2.24127
"FEFF0: feff0005.dat (ifeffit group = feff0_8)"	1.00000	24.16906	0.02572	-8.43947	2.85250	-0.00016	2.85234
"FEFF0: feff0008.dat"	1.00000	2.00000	0.01470	-8.43947	3.51020	-0.01094	3.49926
"FEFF0: feff0009.dat"	1.00000	2.00000	0.00735	-8.43947	3.51580	-0.01094	3.50487
"FEFF0: feff0010.dat"	1.00000	2.00000	0.00367	-8.43947	3.51580	-0.01094	3.50487
"FEFF3: feff0005.dat (ifeffit group = feff3_6)"	1.00000	102.78573	0.06499	-8.43947	3.52570	-0.26680	3.25890

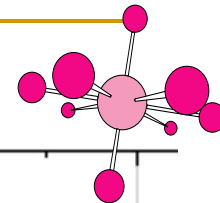
path	ei	3rd	4th	dphase
.....				

Test data for P and Fe shells

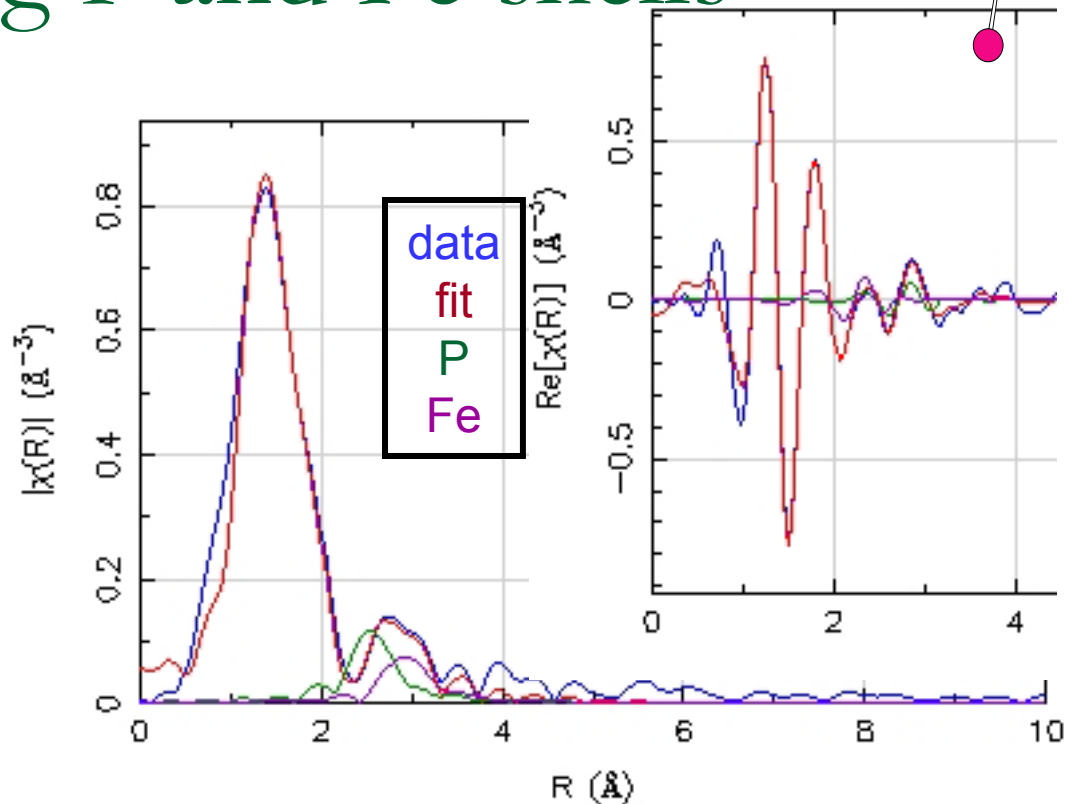


- Place **P** and **Fe** shells in a “good” spot
 - set parameters – no fitting
 - monitor results and fit spectra

Fit Results using P and Fe shells



EXAFS Parameters	
σ^2 -values	-
Distances	+
Coordination numbers	+
ΔE -value	+



Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

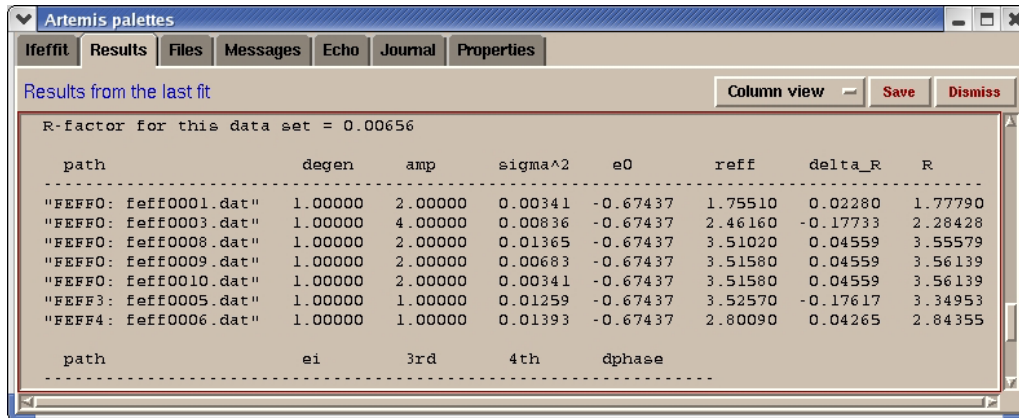
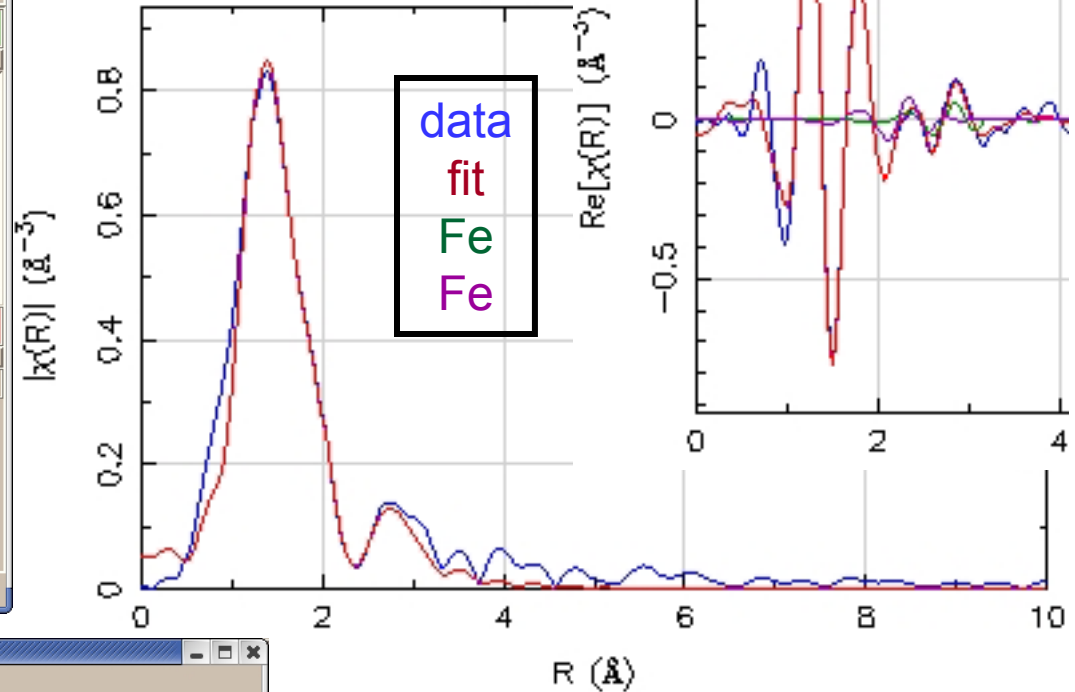
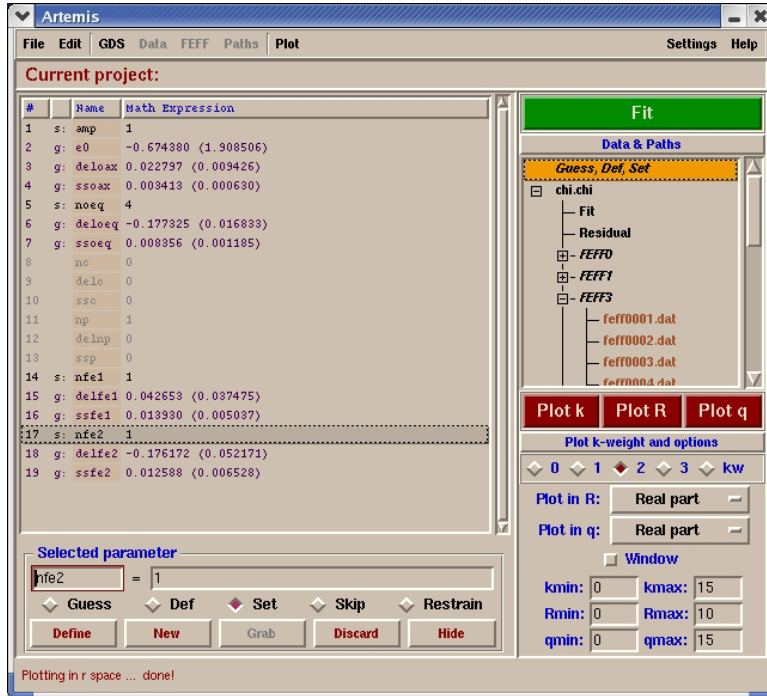
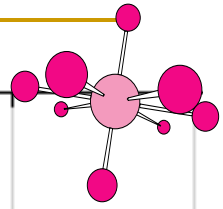
Results from the last fit

Column view Save Dismiss

path	degen	amp	sigma ²	e0	reff	delta_R	R
"FEFF0: feff0001.dat"	1.00000	2.00000	0.00325	1.50997	1.75510	0.03159	1.78669
"FEFF0: feff0003.dat"	1.00000	3.91215	0.00828	1.50997	2.46160	-0.16189	2.29971
"FEFF0: feff0008.dat"	1.00000	2.00000	0.01301	1.50997	3.51020	0.06318	3.57338
"FEFF0: feff0009.dat"	1.00000	2.00000	0.00650	1.50997	3.51580	0.06318	3.57898
"FEFF0: feff0010.dat"	1.00000	2.00000	0.00325	1.50997	3.51580	0.06318	3.57898
"FEFF1: feff0008.dat (lfeffit group = feff1_9)"	1.00000	0.47662	-0.00067	1.50997	3.05550	0.02090	3.07640
"FEFF3: feff0005.dat (lfeffit group = feff3_6)"	1.00000	0.28757	-0.00021	1.50997	3.52570	-0.11686	3.40884

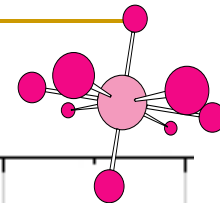
path	e1	3rd	4th	dphase
"FEFF0: feff0001.dat"	0.00000	0.00000	0.00000	0.00000

Test data for Fe and Fe shells

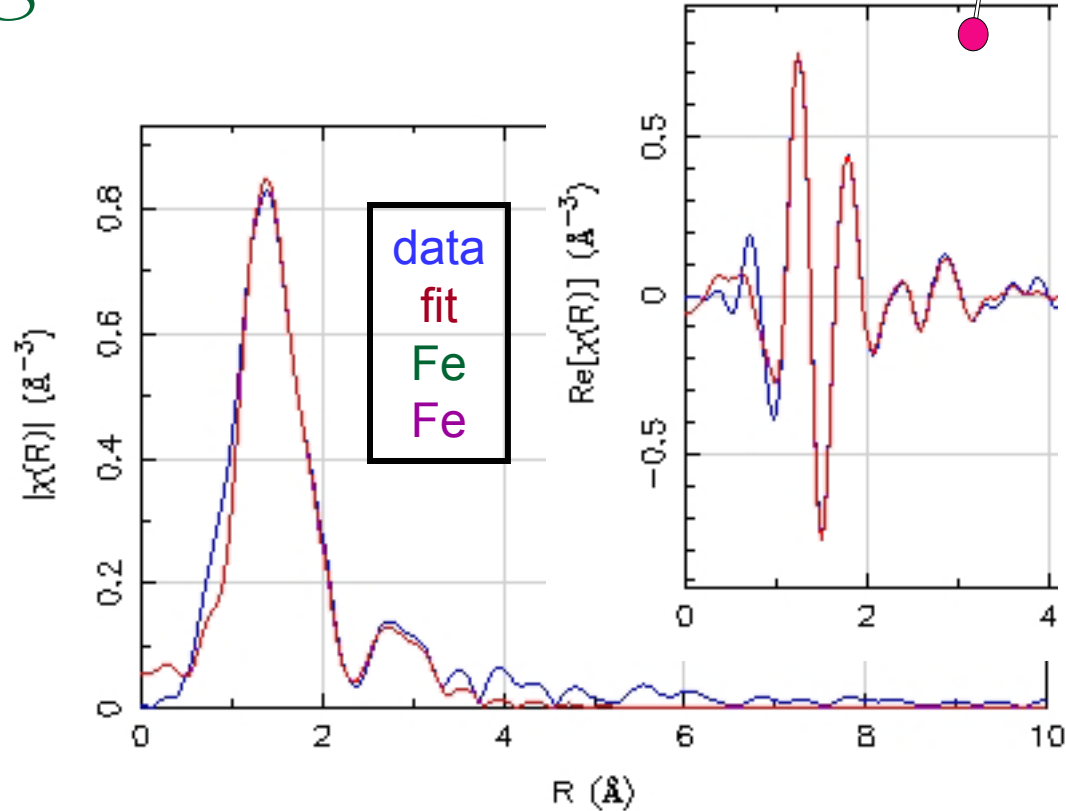


- Place Fe and Fe shells in a "good" spot
 - set parameters – no fitting
 - monitor results and fit spectra

Fit Results using Fe and Fe shells



EXAFS Parameters	
σ^2 -values	+
Distances	+
Coordination numbers	+
ΔE -value	+



Artemis palettes

ifeffit Results Files Messages Echo Journal Properties

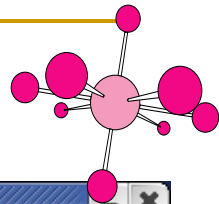
Results from the last fit

phase correction = none

R-factor for this data set = 0.00322

path	degen	amp	sigma^2	e0	reff	delta_R	R
"FEFF0: feff0001.dat"	1.00000	2.00000	0.00324	0.81093	1.75510	0.02730	1.78240
"FEFF0: feff0003.dat"	1.00000	3.43849	0.00669	0.81093	2.46160	-0.16987	2.29173
"FEFF0: feff0008.dat"	1.00000	2.00000	0.01295	0.81093	3.51020	0.05460	3.56480
"FEFF0: feff0009.dat"	1.00000	2.00000	0.00647	0.81093	3.51580	0.05460	3.57040
"FEFF0: feff0010.dat"	1.00000	2.00000	0.00324	0.81093	3.51580	0.05460	3.57040
"FEFF3: feff0005.dat (ifeffit group = feff3_6)"	1.00000	2.10627	0.01908	0.81093	3.52570	-0.14299	3.38271
"FEFF4: feff0006.dat (ifeffit group = feff4_7)"	1.00000	0.39560	0.00560	0.81093	2.80090	0.05323	2.85413

Multiple data set fit



- 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 2nd and 3rd shells

Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project: /home/skelly/Xafs/U/ECM/aug03/fits/artemis1.apj

#	Name	Math Expression
1	s: amp	1
2	g: e0	-0.674373 (1.908498)
3	g: deloax	0.022797 (0.009426)
4	g: ssoax	0.003413 (0.000630)
5	g: noeq	4
6	g: deloeg	-0.177325 (0.016833)
7	g: ssoeg	0.008356 (0.001185)
8	g: delife1	0.042653 (0.037475)
9	g: ssfe1	0.013930 (0.005037)
10	g: delife2	-0.176174 (0.052167)
11	g: ssfe2	0.012587 (0.006528)
12	g: nfe1a	1
13	g: nfe1b	1
14	g: nfe1c	1
15	g: nfe1d	1
16	g: nfe2a	1
17	g: nfe2b	1
18	g: nfe2c	1
19	g: nfe2d	1

Fit

Data & Paths

Guess, Def, Set

- fe1m2
- fe1m1
- fe1m3
- fe2m1
 - FEFF11
 - FEFF12
 - FEFF13

Plot k Plot R Plot q

Plot k-weight and options

0 1 2 3 kw

Plot in R: Real part

Plot in q: Real part

Window

kmin: 0 kmax: 15

Rmin: 0 Rmax: 10

qmin: 0 qmax: 15

Selected parameter

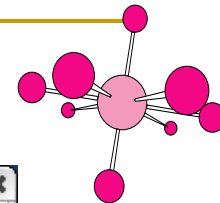
nfe2d = 1

Guess Def Set Skip Restrain

Define New Grab Discard Hide

Defined the guess variable nfe2d as 1

Modeling a Data Series



Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project: /home/skelly/Xafs/U/ECM/aug03/fits/artemis1.apj

#	Name	Math Expression
1	s: amp	1.16631
2	s: deloax	0.042653
3	s: ssoax	0.0047
4	s: noeq	3.443194
5	s: deloeq	-0.103372
6	s: ssoeq	0.010684
7	s: delfe1	0.080562
8	s: ssfe1	0.005210
9	s: delfe2	-0.113842
10	s: ssfe2	ssfe1
11	s: nfe1a	0.476039 (0.2)
12	s: nfe1b	0.508141 (0.2)
13	s: nfe1c	0.554804 (0.3)
14	s: nfe1d	0.579083 (0.3)
15	s: nfe2a	0.637507 (0.2)
16	s: nfe2b	0.450068 (0.2)
17	s: nfe2c	0.475028 (0.3)
18	s: nfe2d	0.637507 (0.3)
19	s: e0c	e0a
20	s: e0a	6.907468
21	s: e0b	e0a
22	s: e0d	e0a

Selected parameter

nfe1d = 0.579083 (0.3)

◆ Guess ◆ Def ◆ Set ◆ Skip ◆ Restrain

Define New Grab Discard Hide

nfe1d = 0.774106 +/- 8.116450

Fit

Data & Paths

Guess, Def, Set

- fe1m1
- fe1m2
- fe1m3
- fe2m1

Plot k Plot R Plot q

Plot k-weight and options

◆ 0 ◆ 1 ◆ 2 ◆ 3 ◆ kw

Plot in R: Real part

Plot in q: Real part

Window

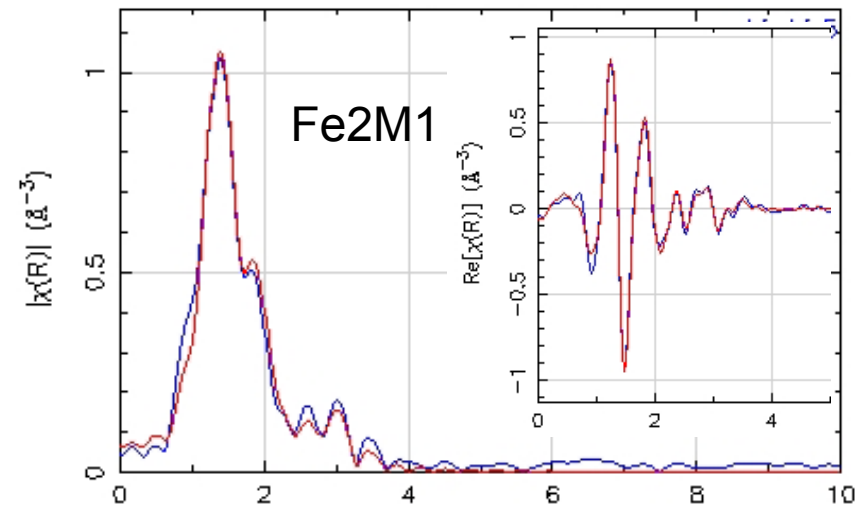
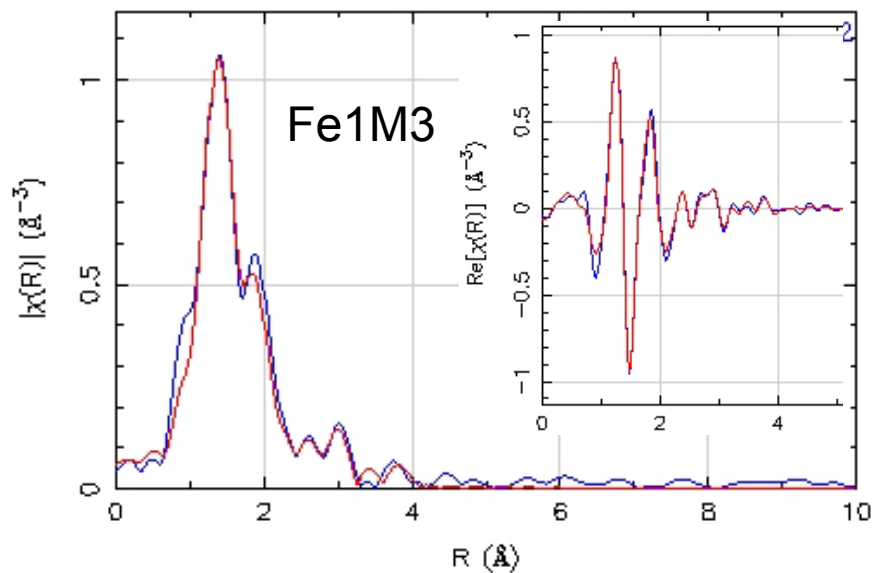
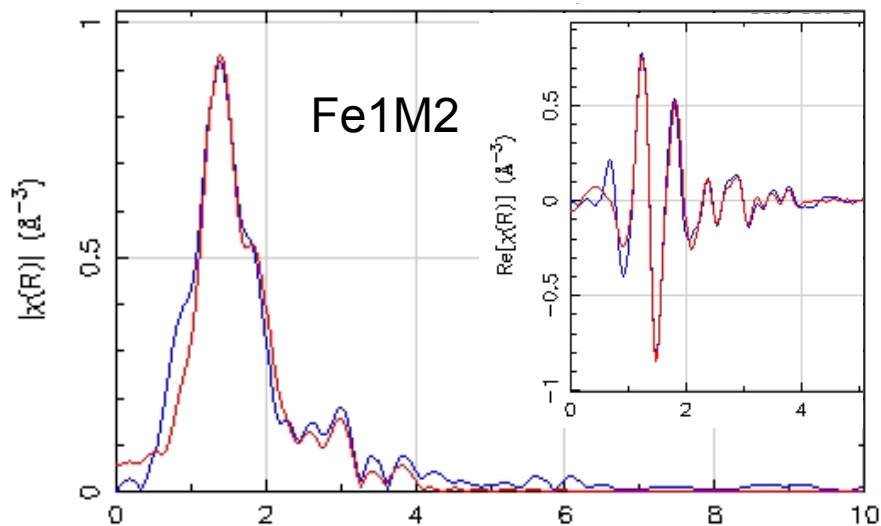
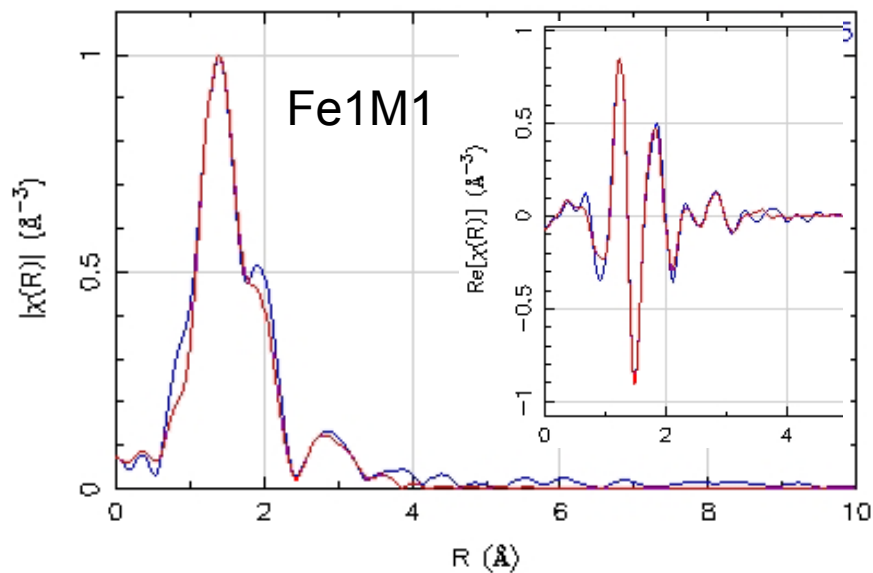
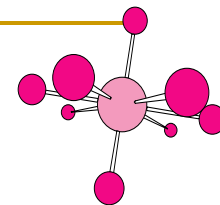
kmin: 0 kmax: 15

Rmin: 0 Rmax: 10

qmin: 0 qmax: 15

- Coordination number is determined within 5%
- Assuming model is accurate!

Fit results from data series



Summary

