Introduction to EXAFS data analysis

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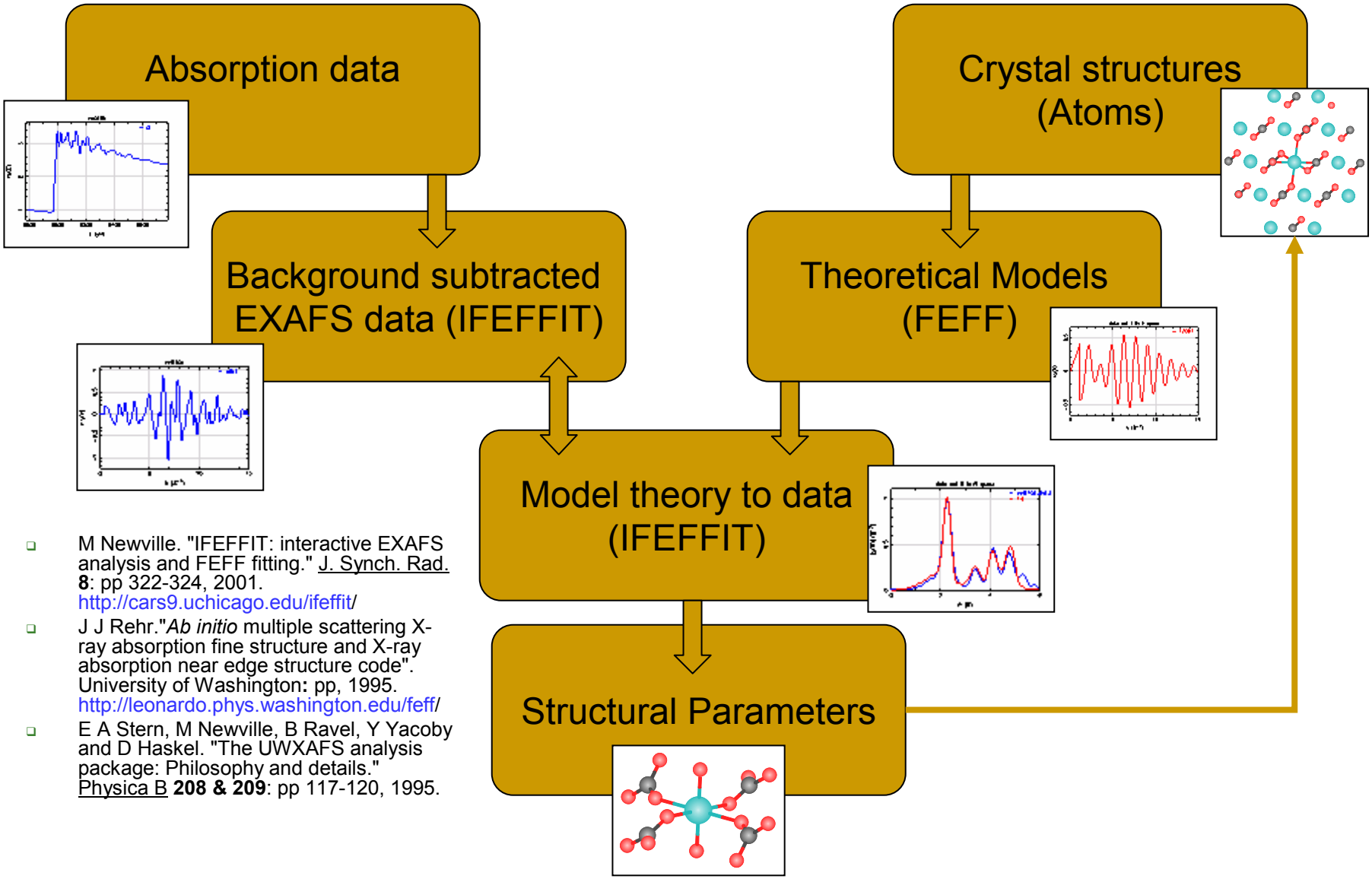
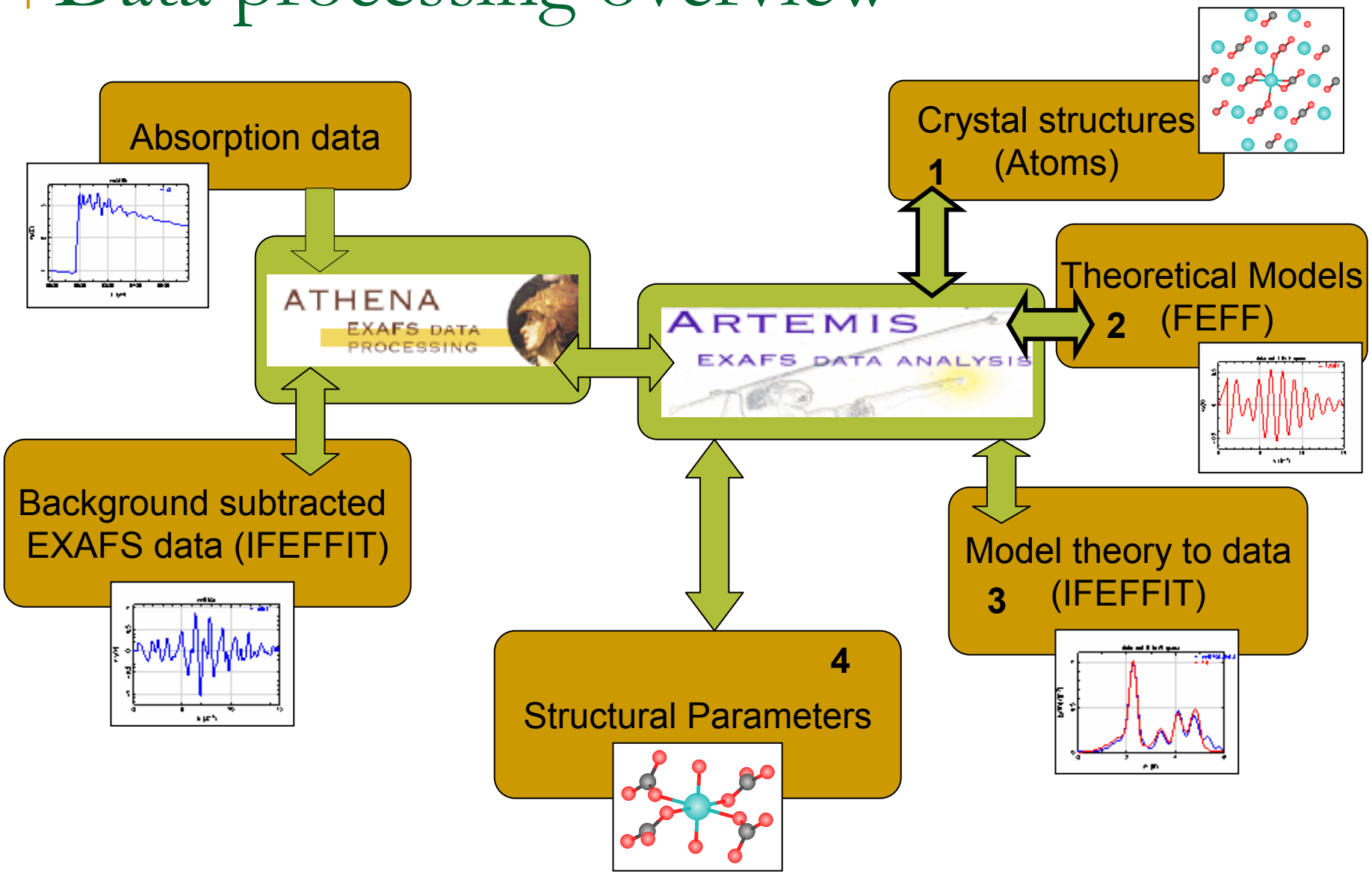
Data processing overview



- 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.

Data processing overview



- http://leonardo.phys.washington.edu/~ravel/software/exafs/

Artemis

Project Name:

Menus:

Fit: optimize variables

Variables

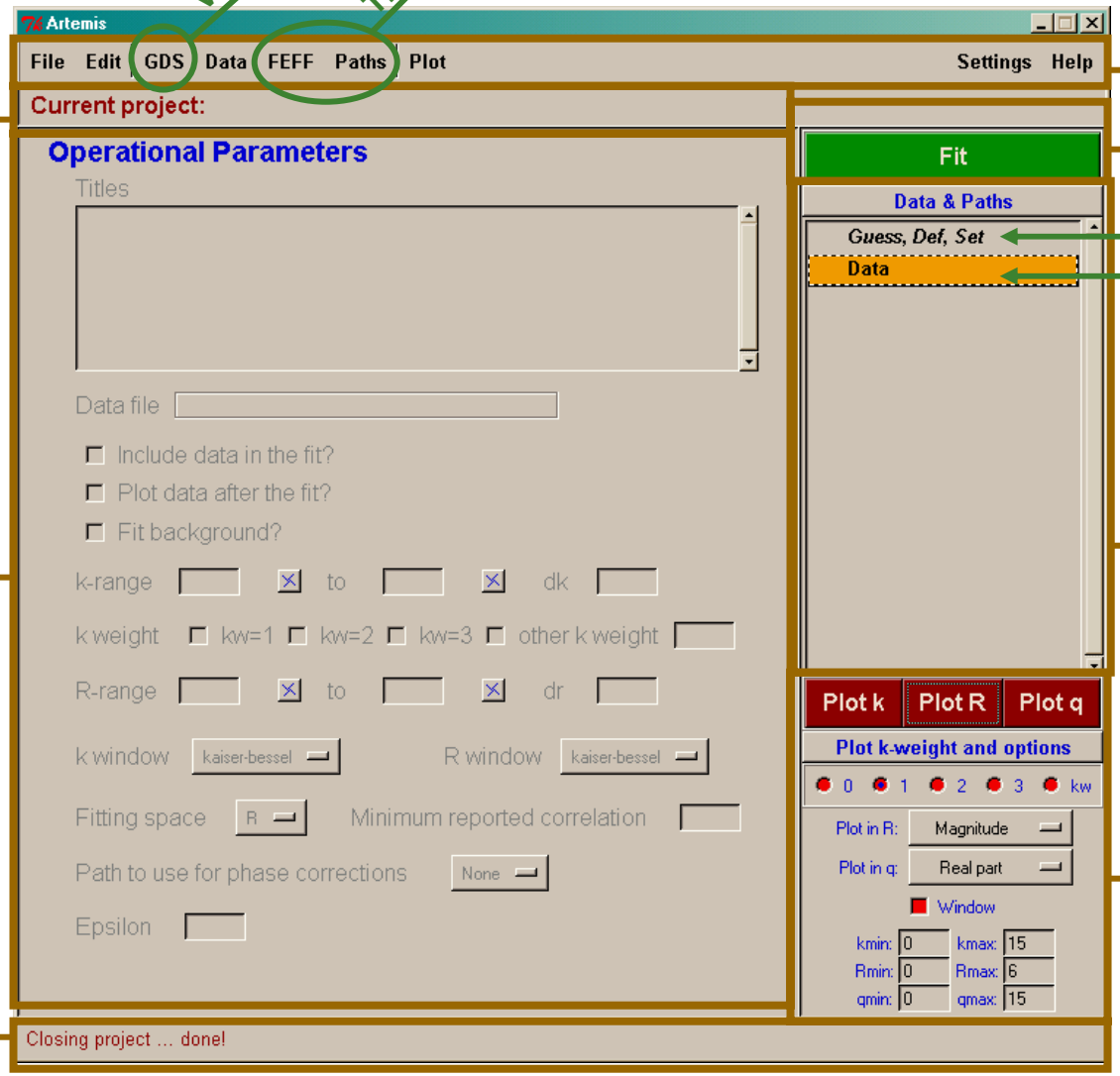
Data: input from Athena

Data display area:
Changes depending on selected information from Data and Paths list

Data and Paths:
Changes data display area

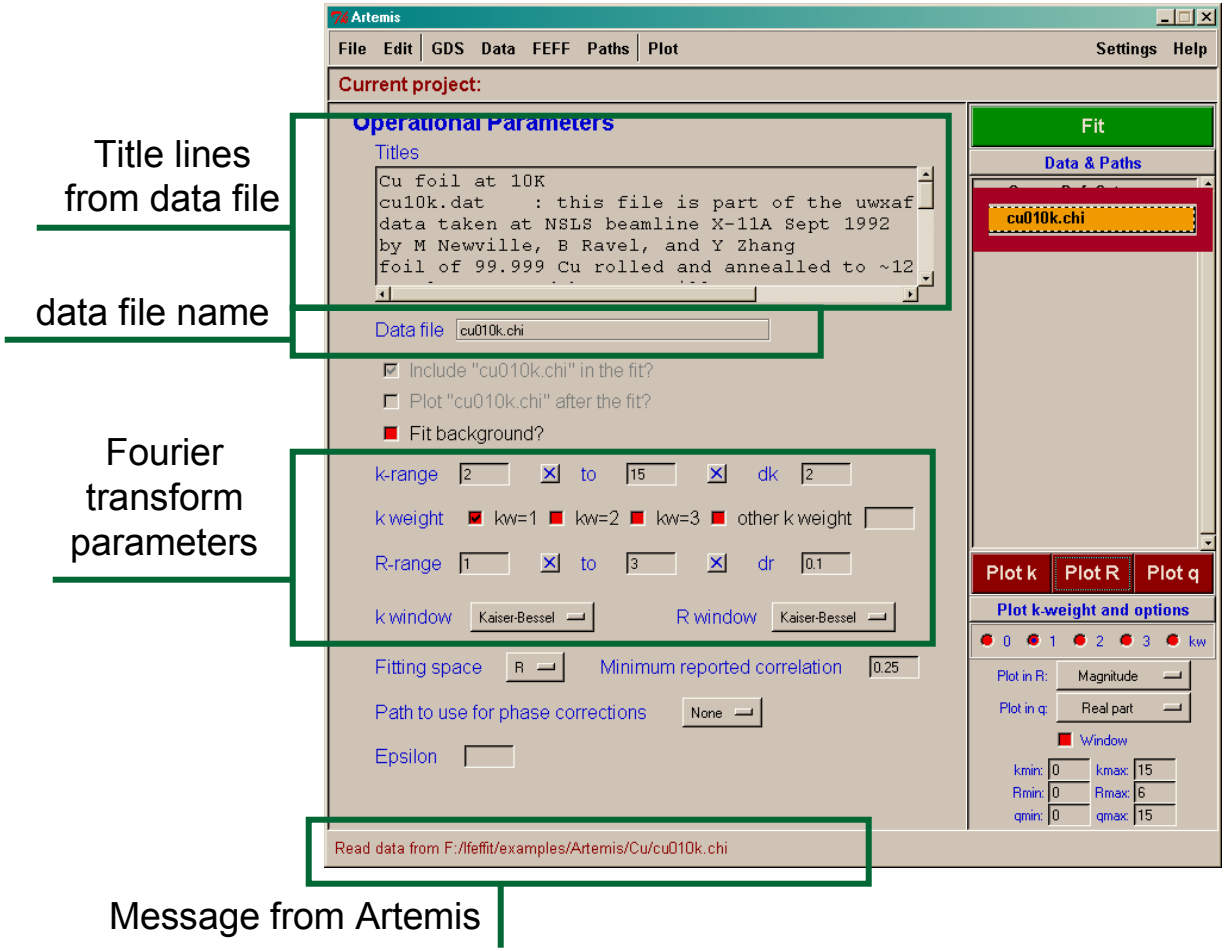
Plotting parameters

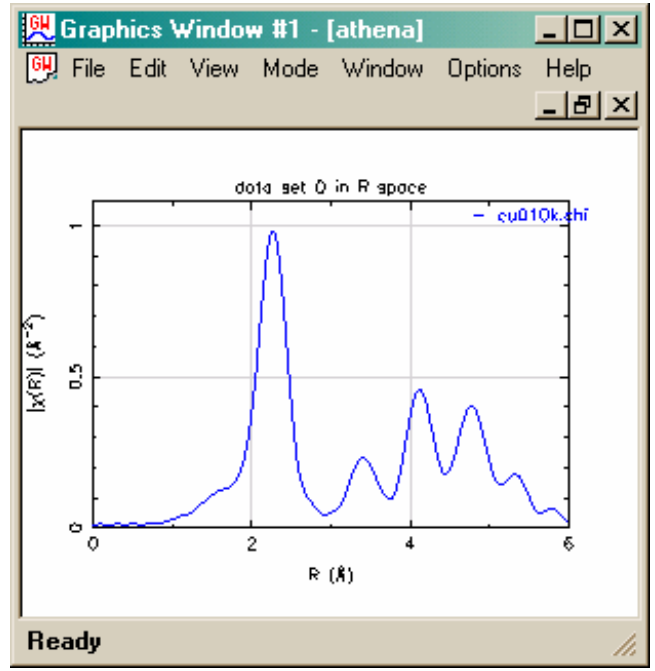
Echo Area:
Messages from Artemis



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

Reading in Data



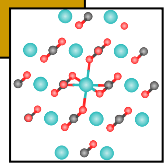


Data plotted in R-space

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

Atoms page

Crystal structures
1 (Atoms)



Title lines

Always much larger than paths used in fit

Structural Information

Atom with a core hole

Absorption edge

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

Message from Artemis

Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project:

Atoms feff.inp Interpretation

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	○					

Run Atoms Add a site

Fit

Data & Paths

Guess, Def, Set

cu010k.chi

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

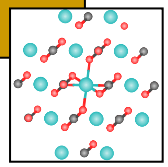
qmin: 0 qmax: 15

Importing atoms.inp file ... done!

➢Click “Run Atoms”

Theory input page (feff.inp)

Crystal structures
1 (Atoms)



absorption lengths

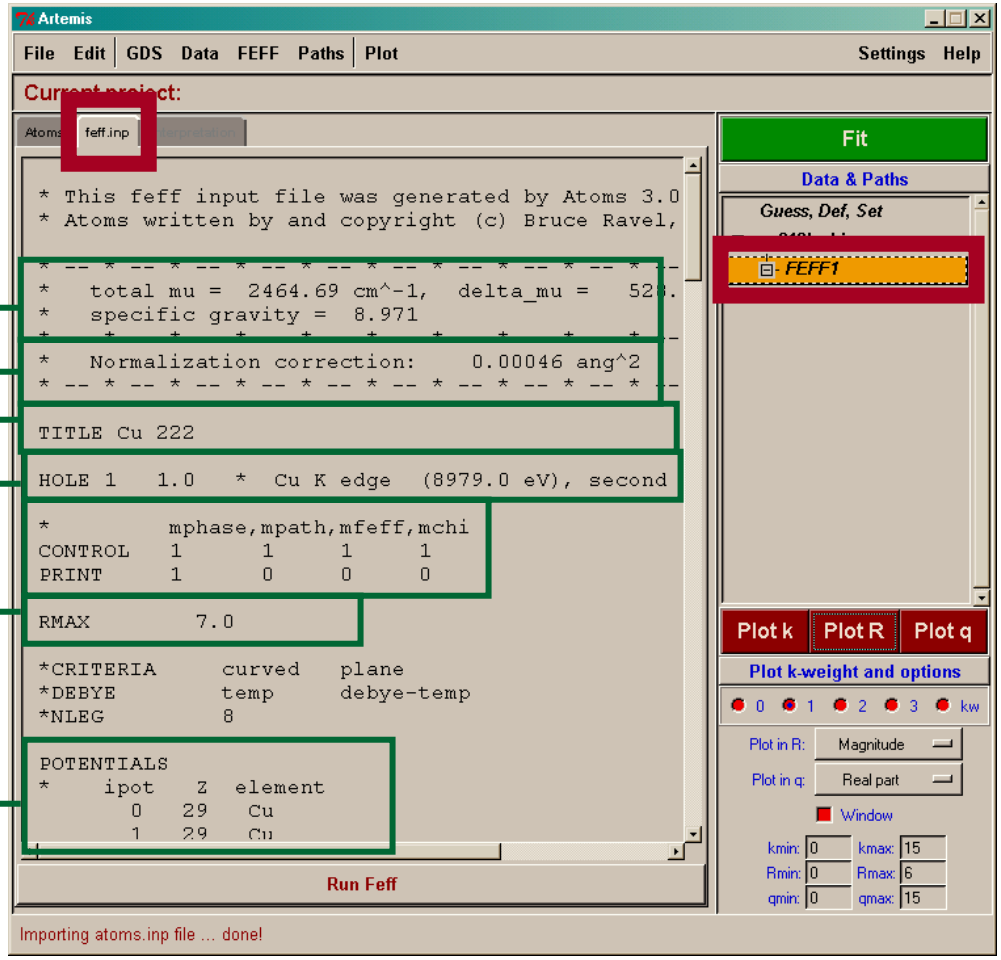
normalization correction

title lines

hole number

max path length

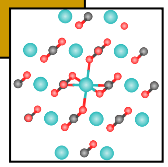
potential list



➢Scroll feff.inp page downward

Theory input page (feff.inp)

Crystal structures
1 (Atoms)

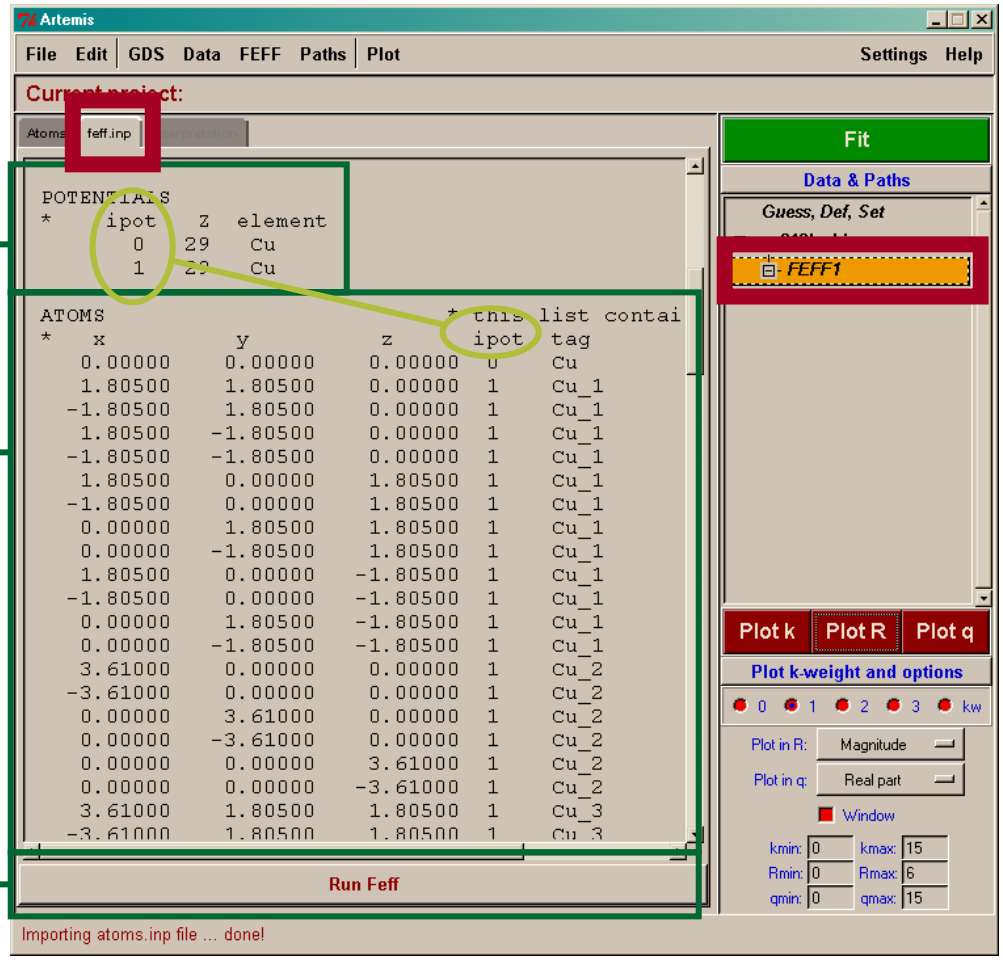


Potential list

Atoms list

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

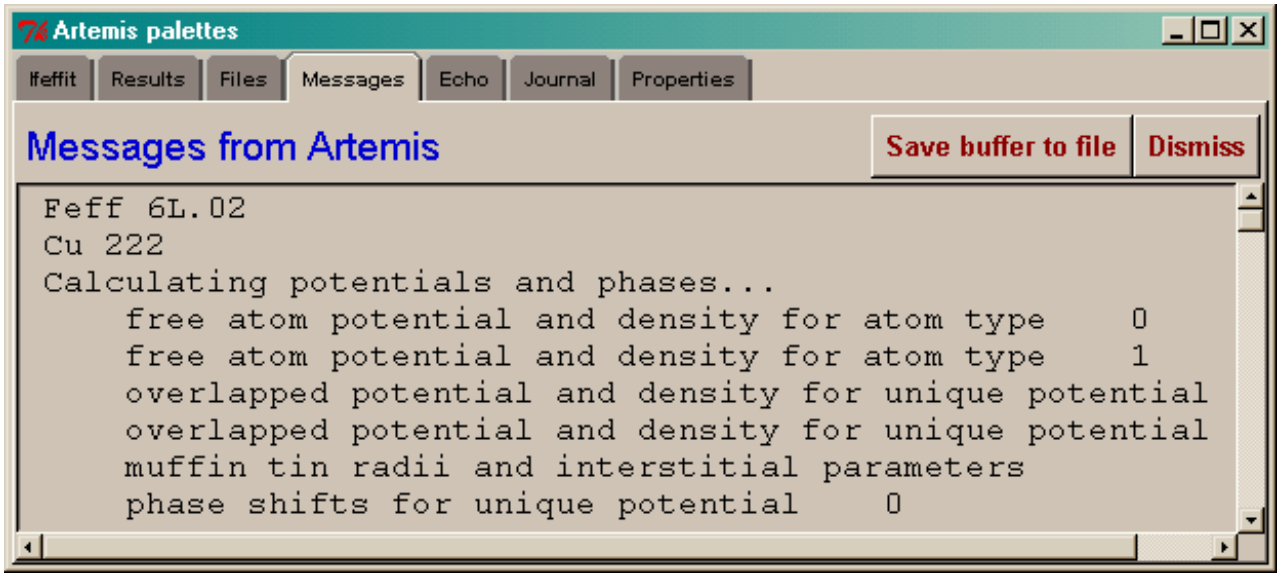
Run Feff



➢Click on Run Feff button

Running Feff

Text messages during Feff calculation

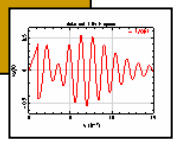


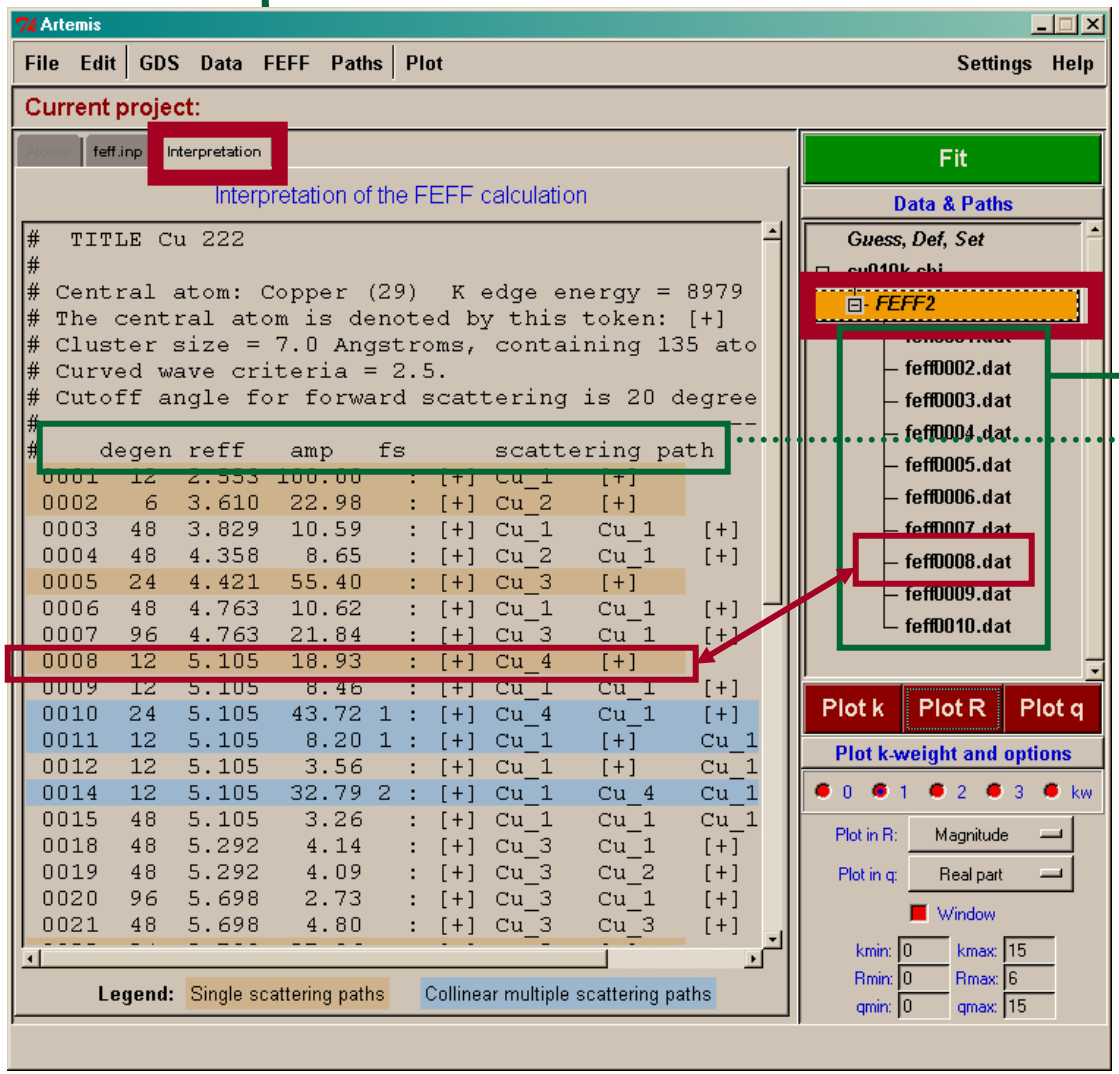
Artemis Palettes

- Ifeffit: Shows the interface from Artemis to Ifeffit. Artemis is just a nice interface to Ifeffit. Ifeffit 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

Theoretical Models
2 (FEFF)





- 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.

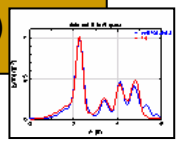
Feff paths

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

Artemis

File Edit GDS Data FEFF Paths Plot Settings Help

Current project:

Path Description

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
```

Path parameter math expressions

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

Fit

Data & Paths

Guess, Def, Set

cu010k.chi

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

0 1 2 3 kw

Plot in R: Magnitude

Plot in q: Real part

Window

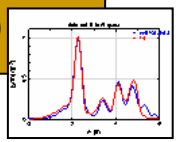
kmin: 0 kmax: 15

Rmin: 0 Rmax: 6

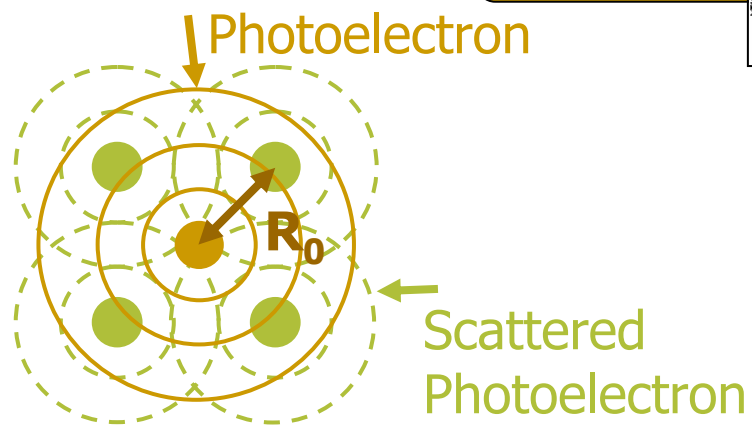
qmin: 0 qmax: 15

The EXAFS Equation

Model theory to data
3 (IFEFFIT)



- E. A. Stern and S M Heald Basic principles and applications of EXAFS. Handbook of Synchrotron Radiaction. 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.



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

with each path written as:

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

$$R_i = R_0 + \Delta R$$

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

Theoretically calculated values

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

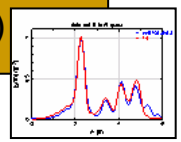
Feff calculates the theoretical scattering amplitude F(k) effective, hence the name Feff.

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

Path Parameters

Model theory to data
3 (IFEFFIT)



- 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.

Parameters often determined from a fit to data

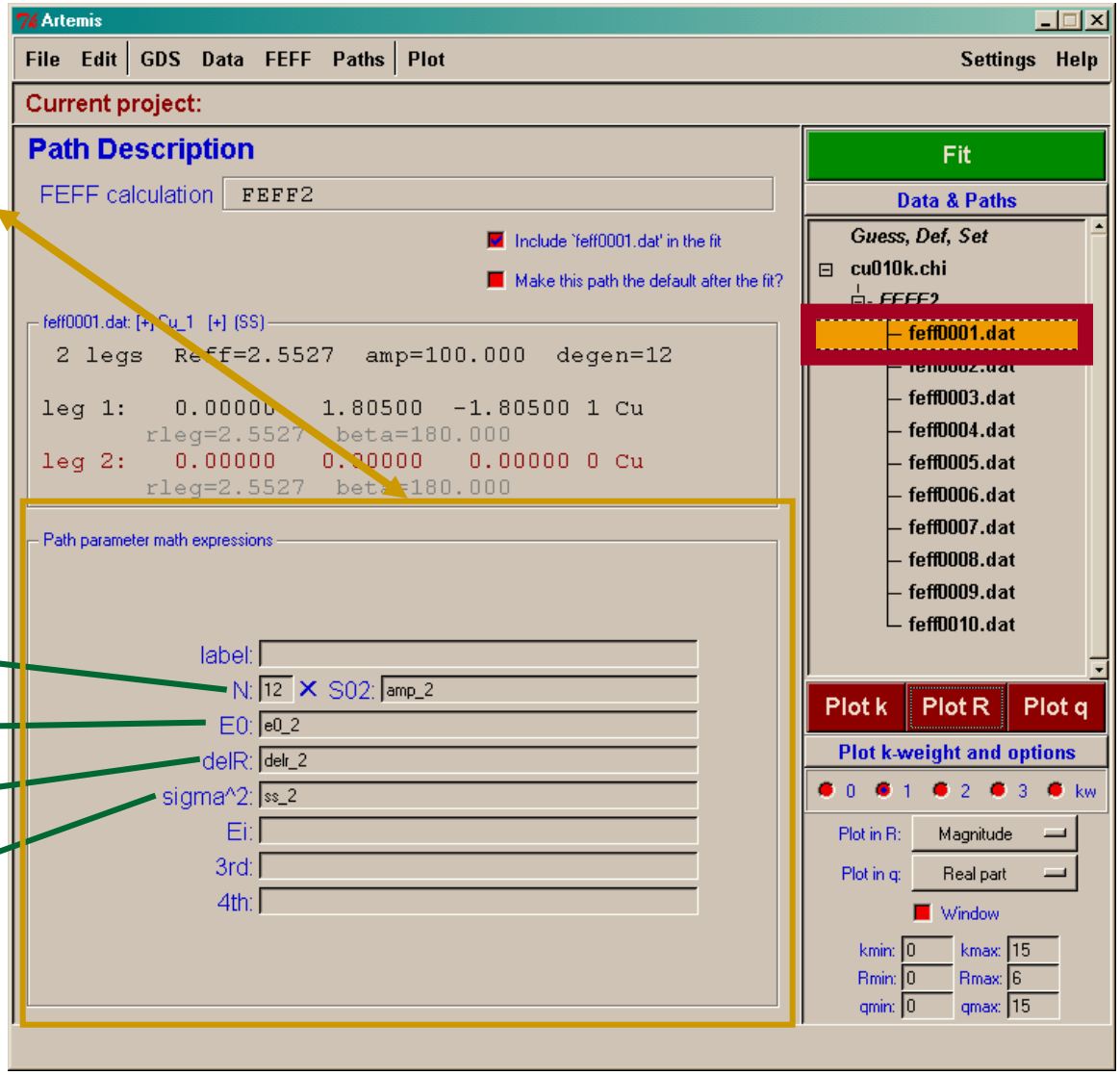
S02 passive electron reduction factor

N degeneracy of path

E0 energy shift

delR change in half-path length

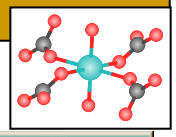
sigma^2 mean squared displacement



➢Click “Guess, Def, Set” in the Data & Paths list

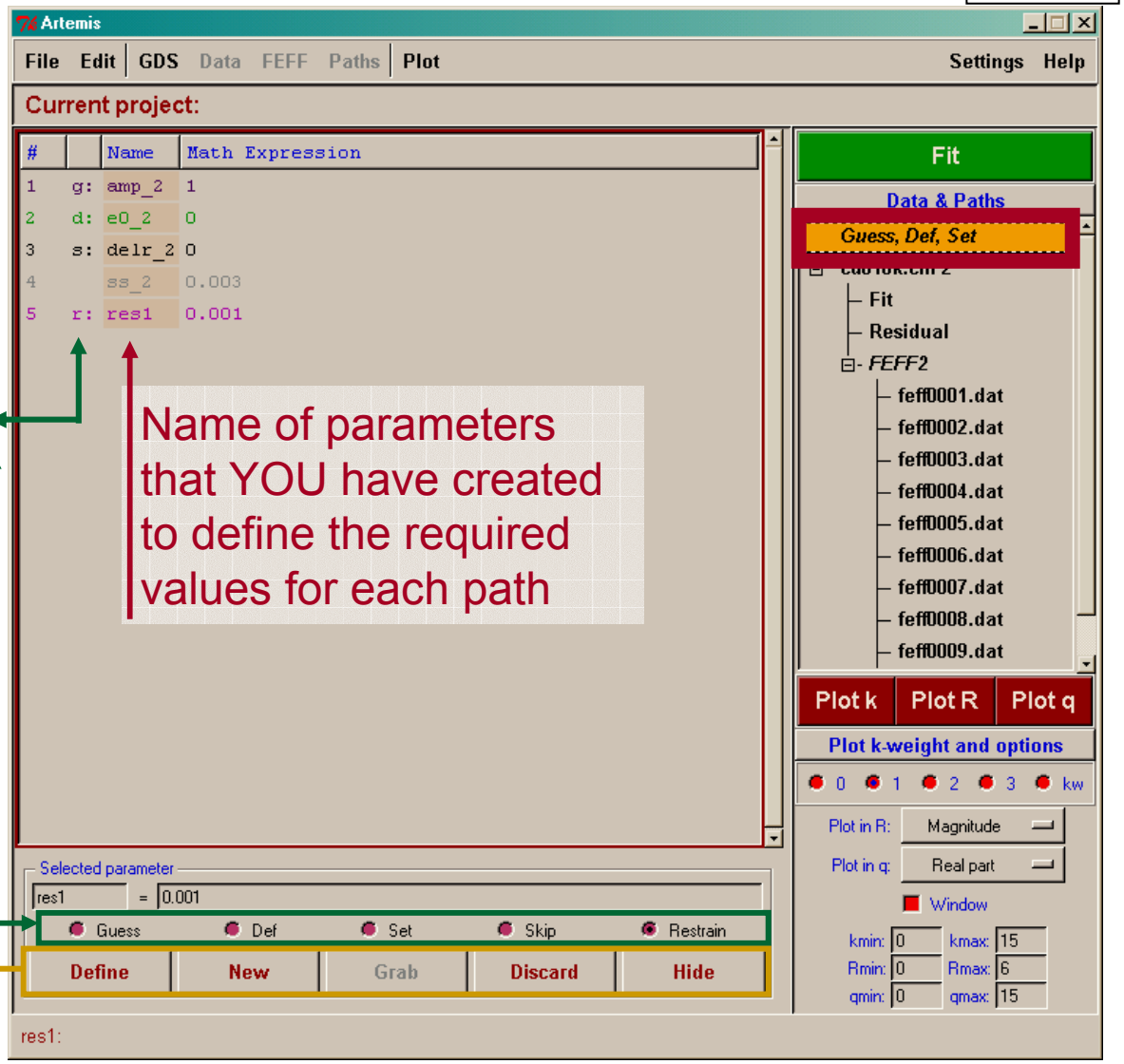
EXAFS parameters

4
Structural 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.

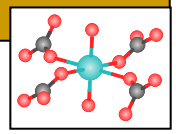
- Define: Define parameter to value given.
- New: Make a new parameter.
- Grab: Set the value to the best-fit value from the fit.
- Discard: remove parameter.
- Hide: Hide editing area



➢Click "Fit" to optimize these values

Fit Results

4
Structural Parameters



Artemis palettes

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

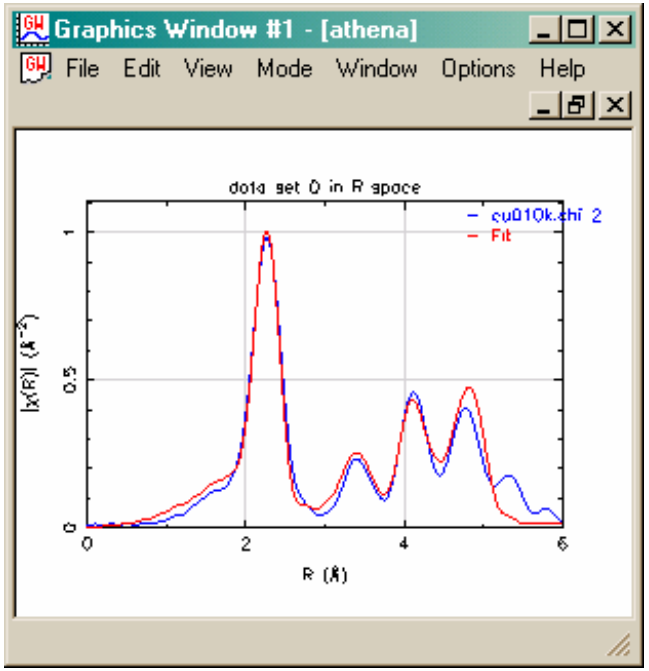
Results from the last fit

Raw log file | Save | Dismiss

```
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           =      16.187500000
Number of variables          =       4.000000000
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:
    amp_2 and ss_2          -->  0.8842
    amp_2 and delr_2        -->  0.7957
All other correlations are below 0.25
```

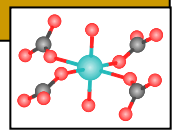
Your parameters

Initial guessed value



➢Scroll down

Fit Results



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

Artemis palettes

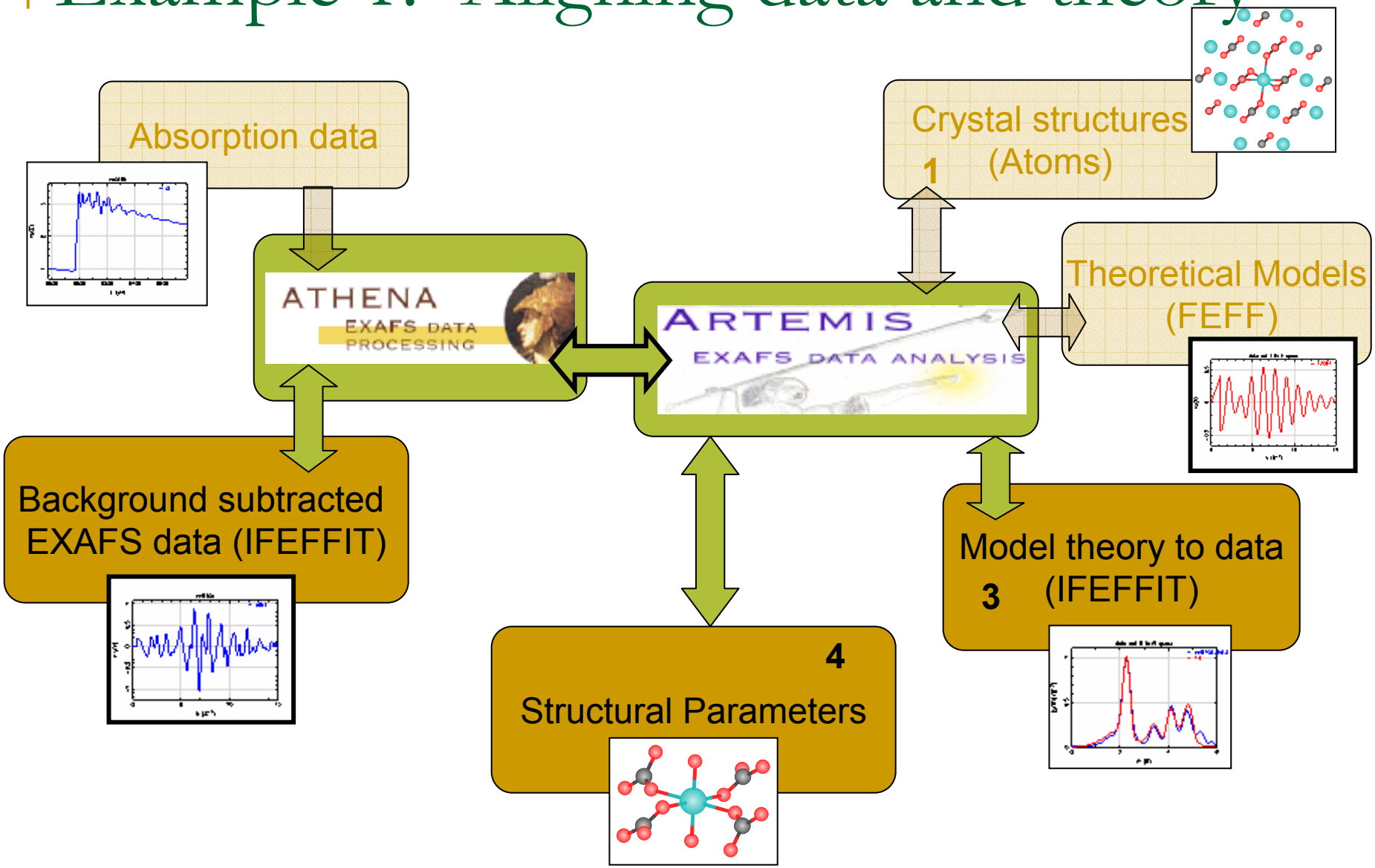
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit

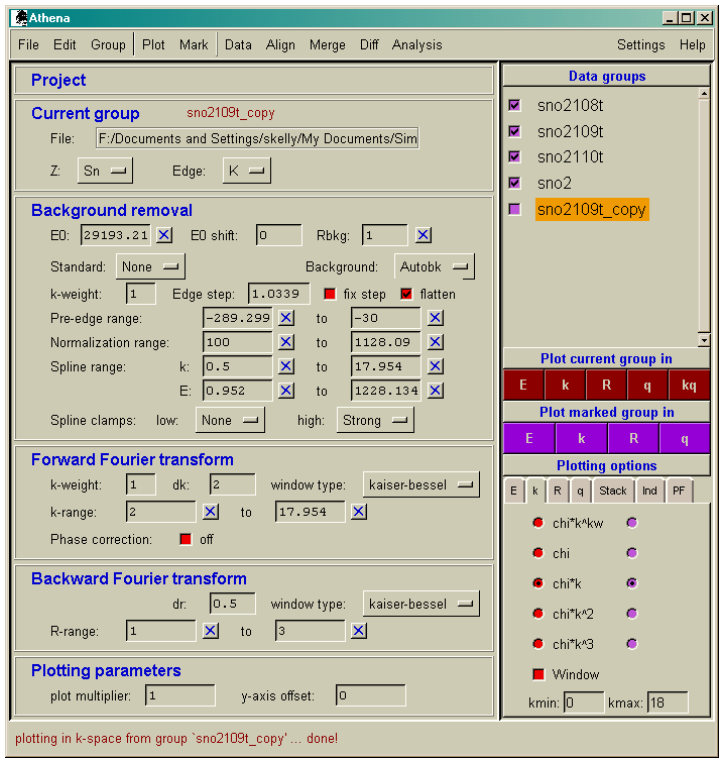
Raw log file | Save | Dismiss

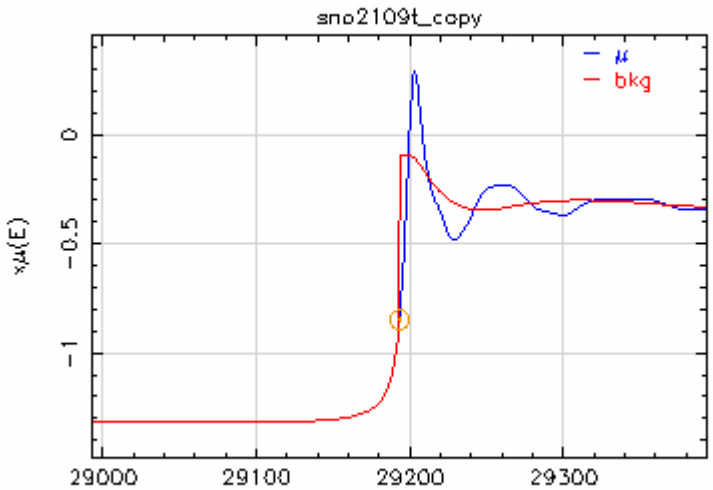
```
===== Paths used to fit cu010k.chi 2

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
```

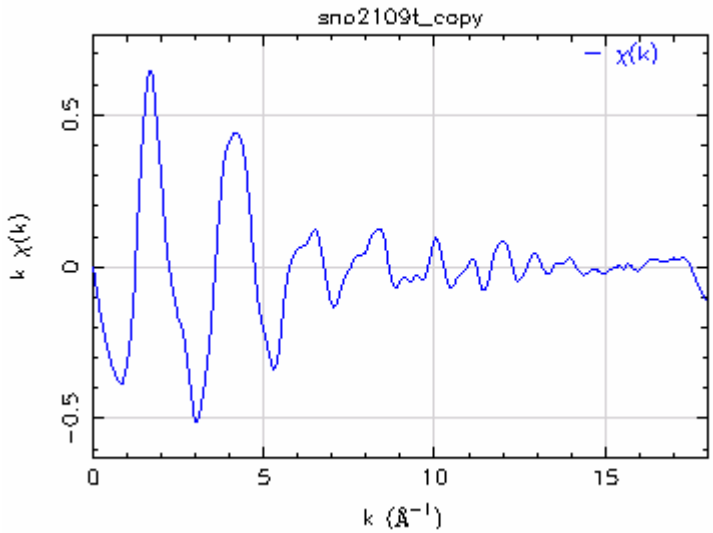
Example 1: Aligning data and theory



SnO_2 first background removal from Athena



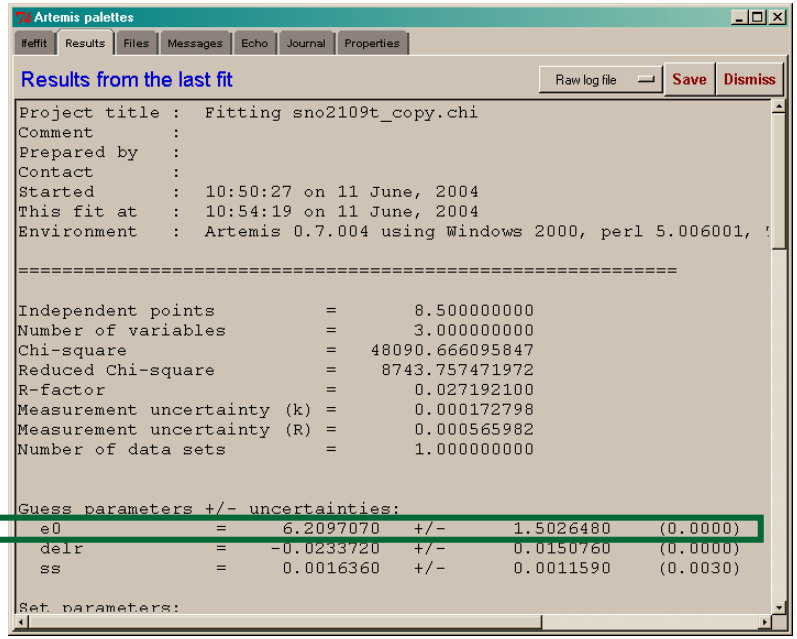


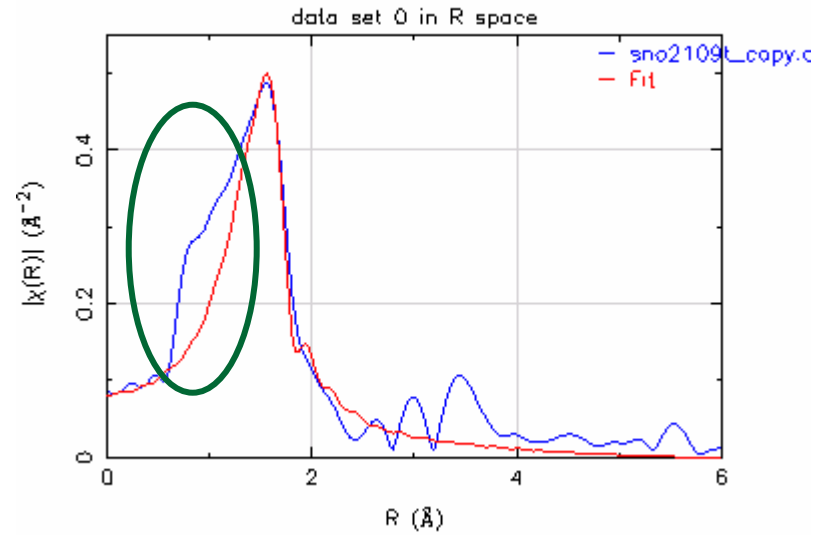


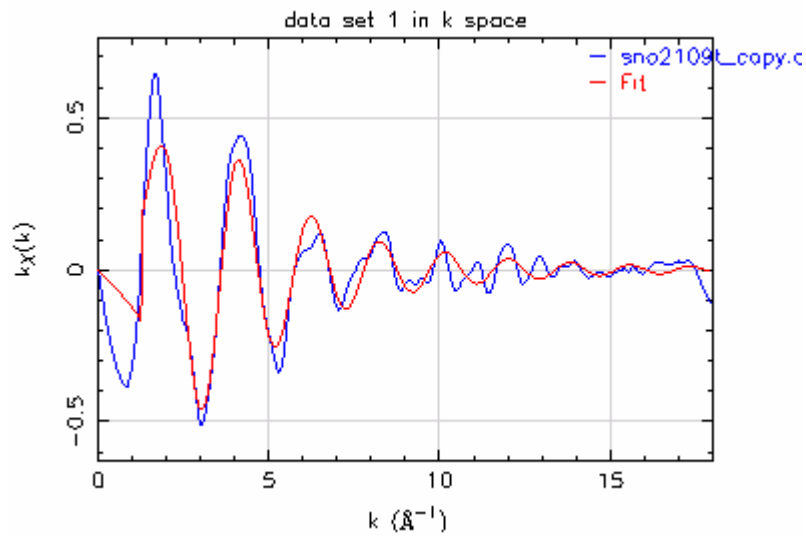
- E0 is somewhere on the edge
- Using default parameters

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

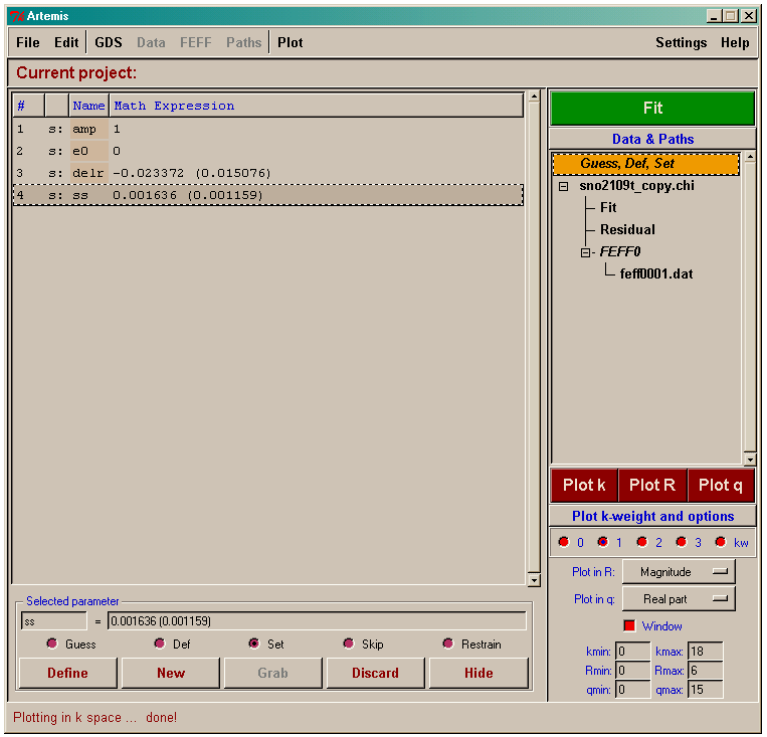


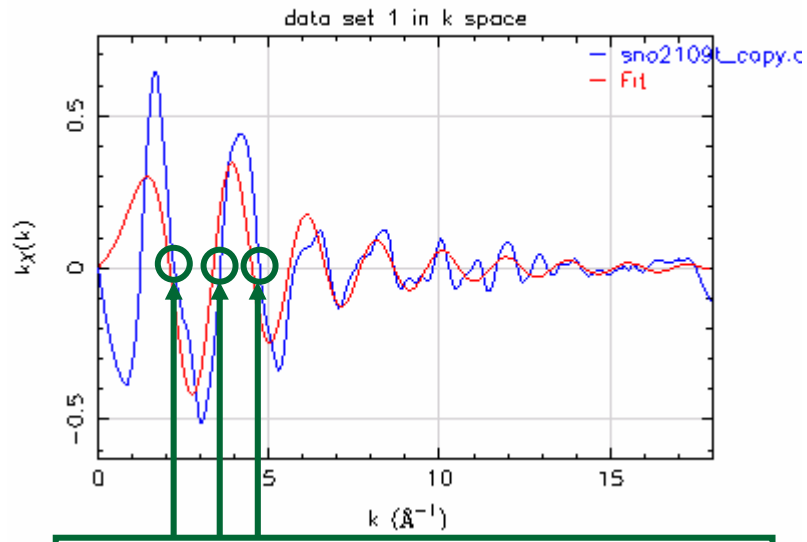




- E0 could be smaller
- Background needs to be adjusted
- More information: M Newville, B Ravel, D Haskel and E A Stern. "Analysis of multiple scattering XAFS data using theoretical standards." Physica B **208 & 209**: pp 154-156, 1995.

Create first shell model with E0=0

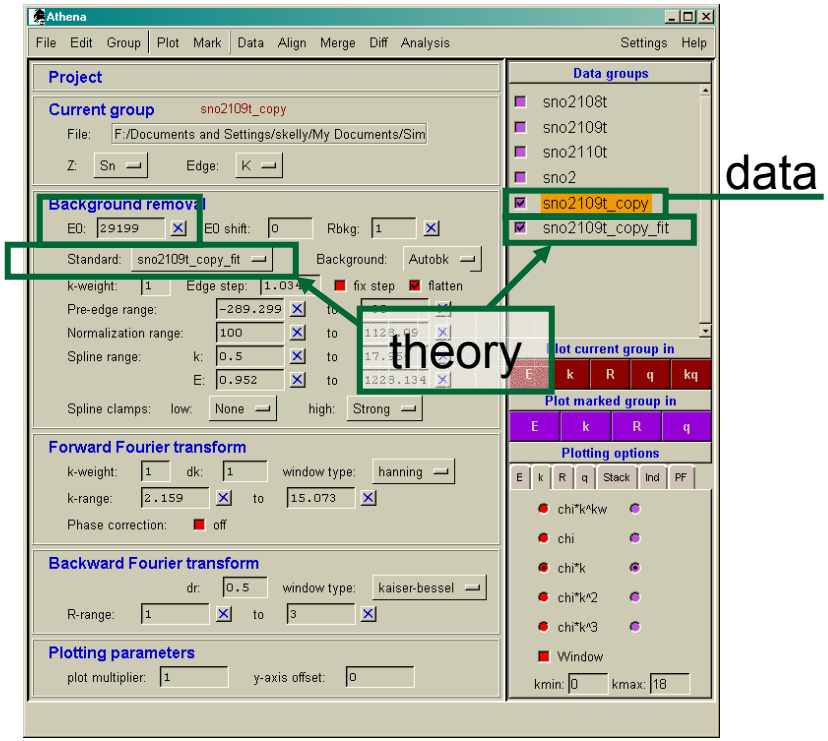


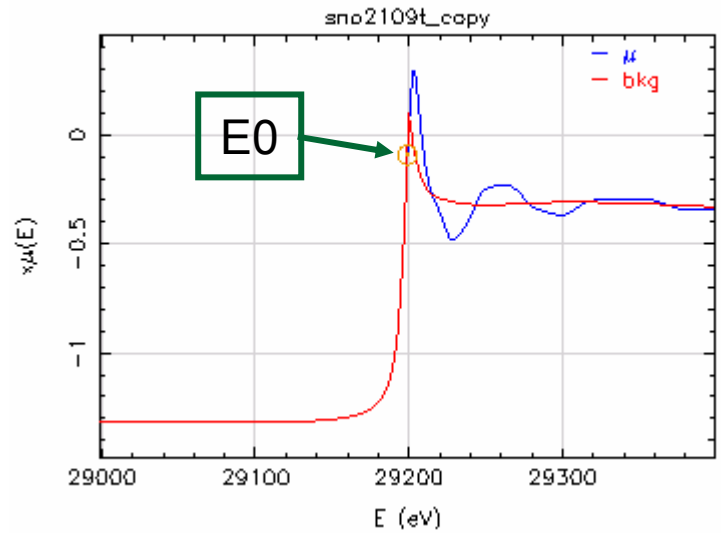


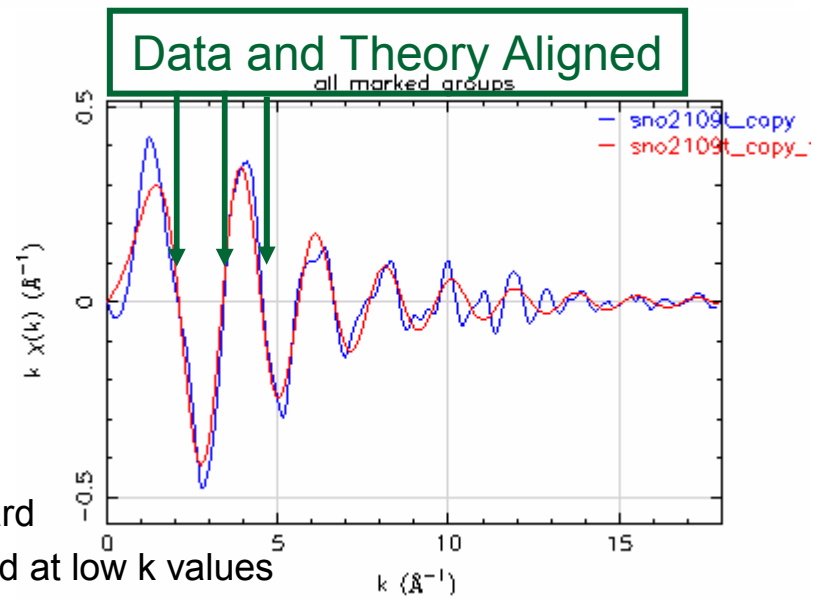
Data and theory are not aligned

- Set parameters to their best-fit values by using the Grab button.
- Change all parameters from guess to set.
- Set E0=0.
- Run the “Fit” again to produce the theory with zero for E0.

Background corrected and energy aligned by using theory

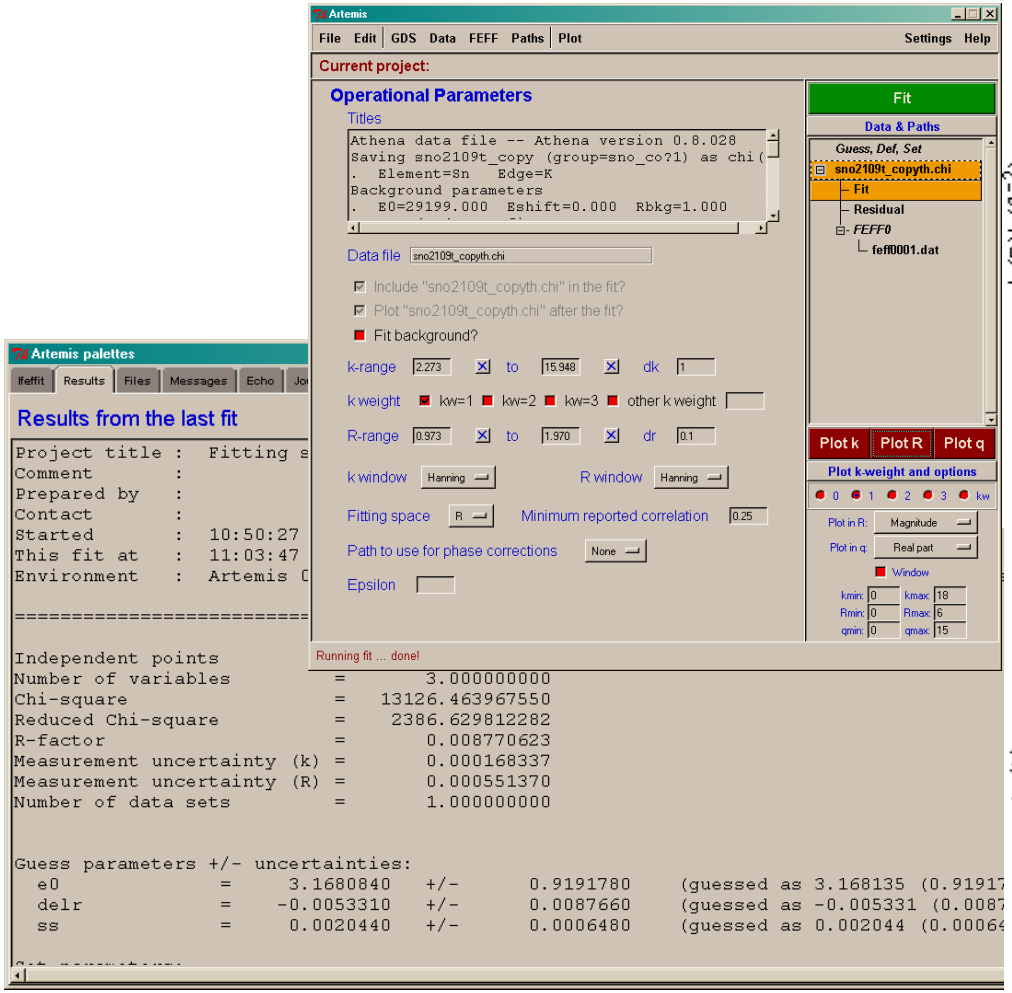


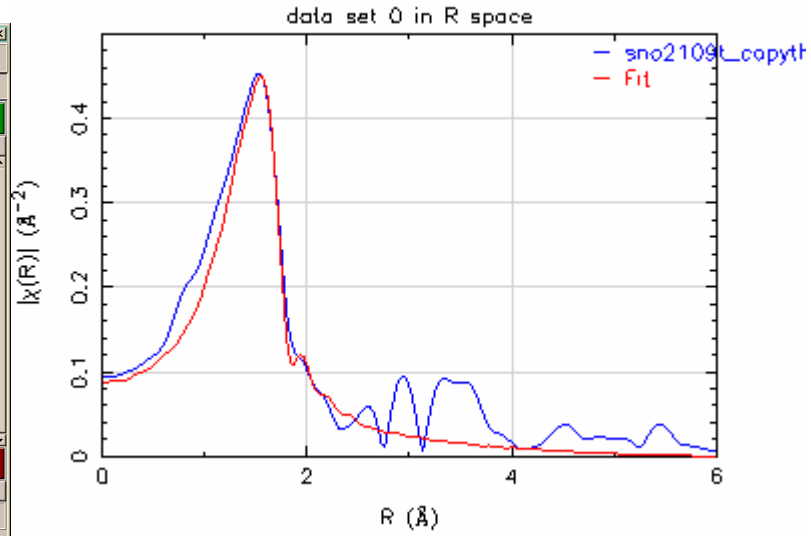


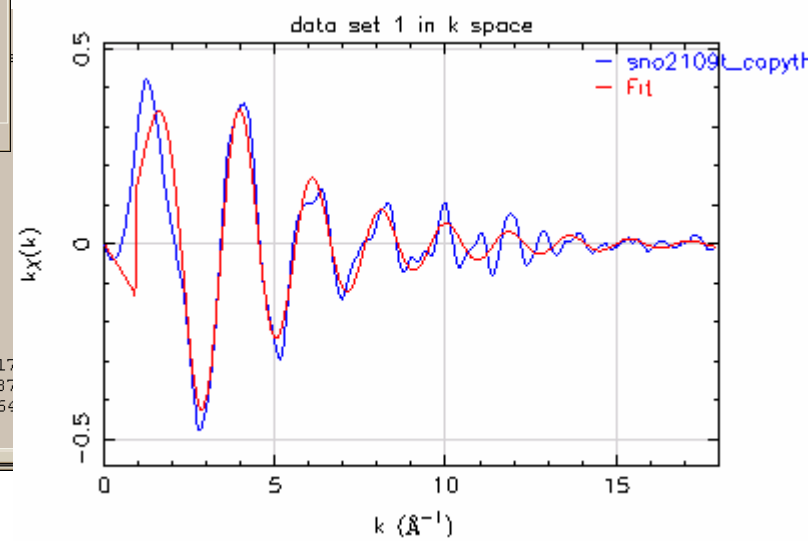


- Read the theory into Athena
- Select your data and use the theory as a standard
- Adjust E0 so that the data and theory are aligned at low k values

Fit to first shell with background adjusted

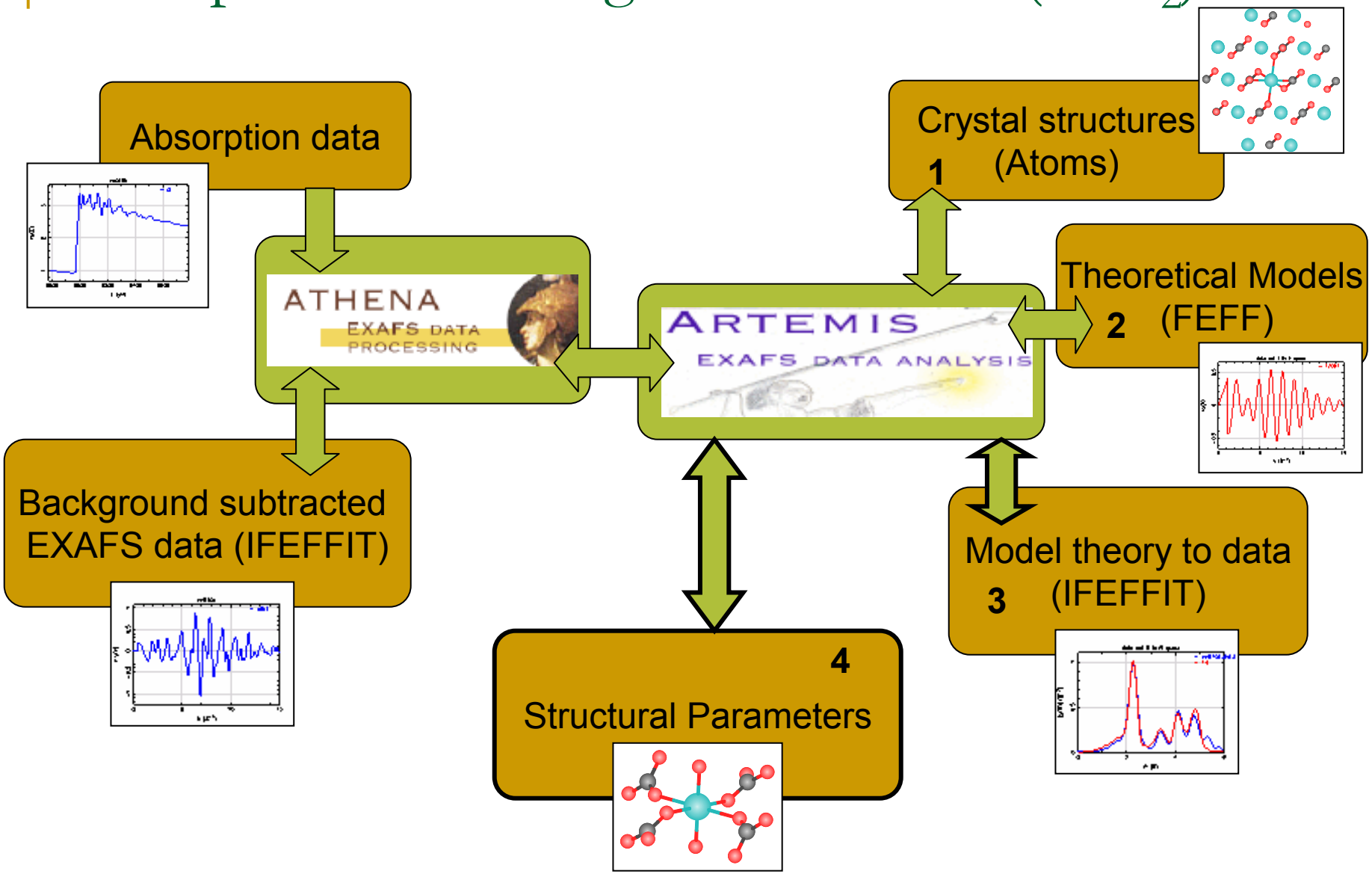




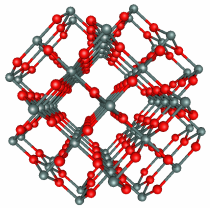


- Read the chi(k) data back into Artemis and fit the first shell

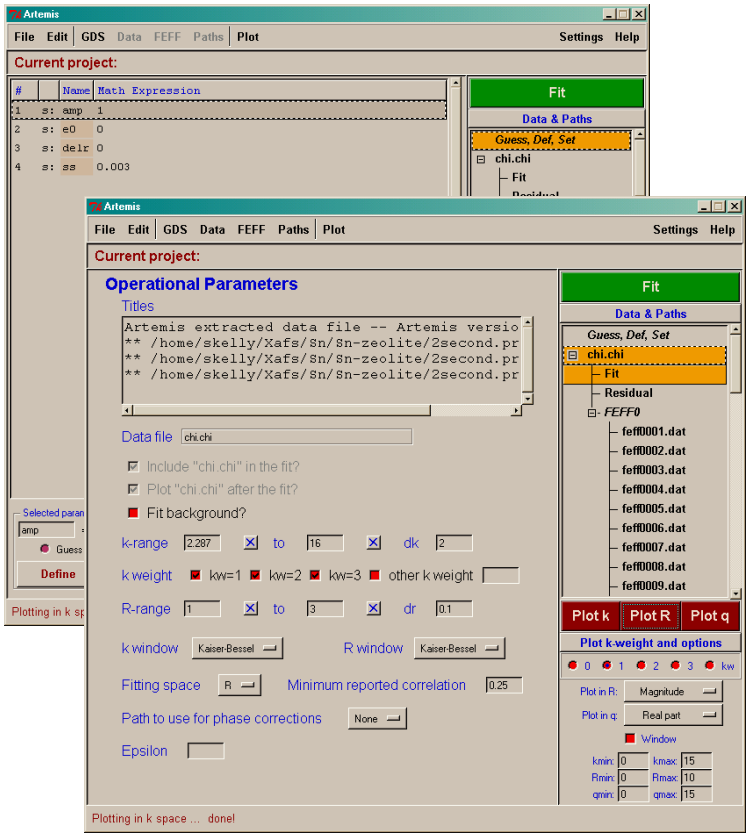
Example 2: Modeling a metal-oxide (SnO_2)

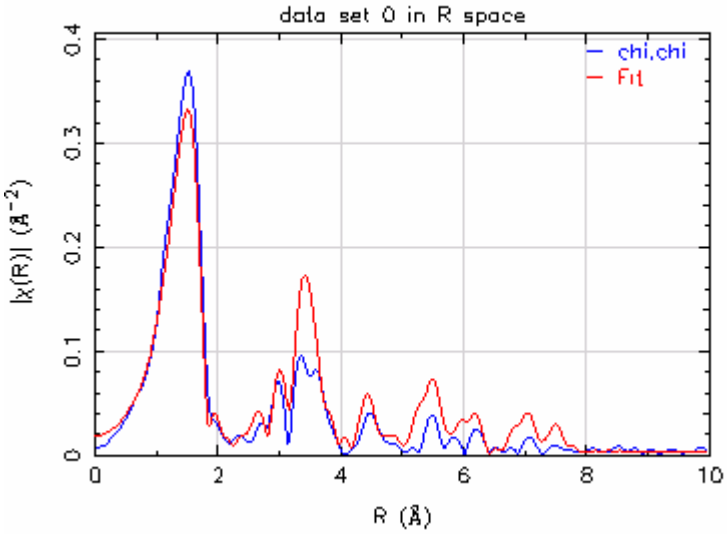


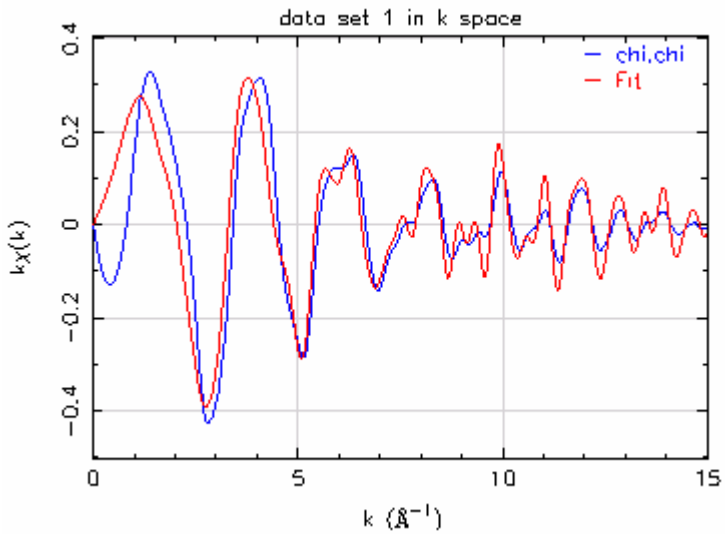
Example 3: Modeling a metal-oxide (SnO_2)



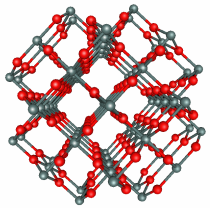
- Compare the sum of all 69 paths to the data



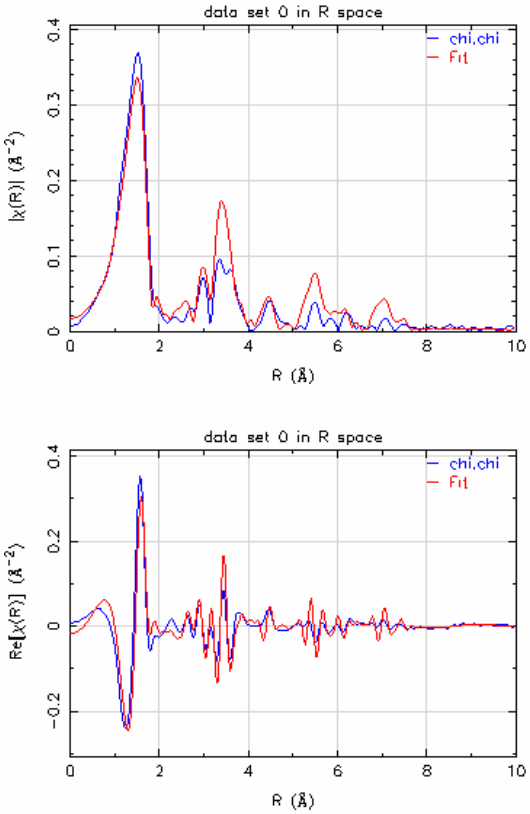




How many paths are required?

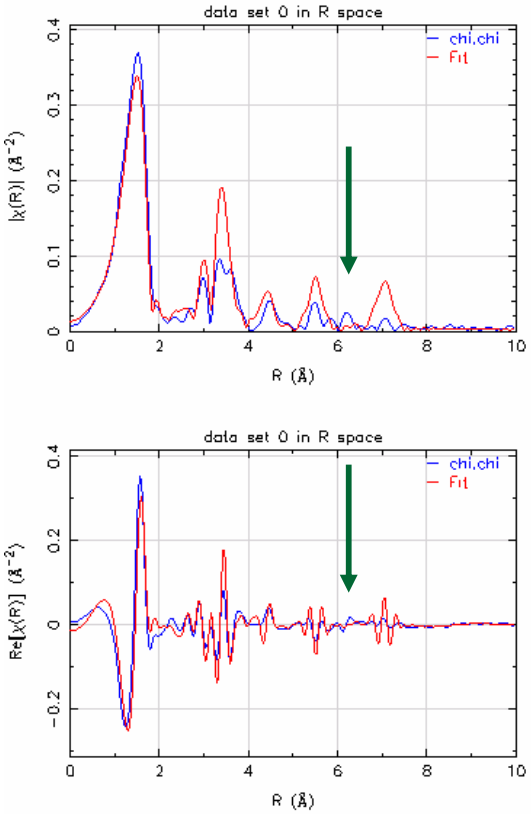


Minimum amplitude 5%
30 of 69 paths



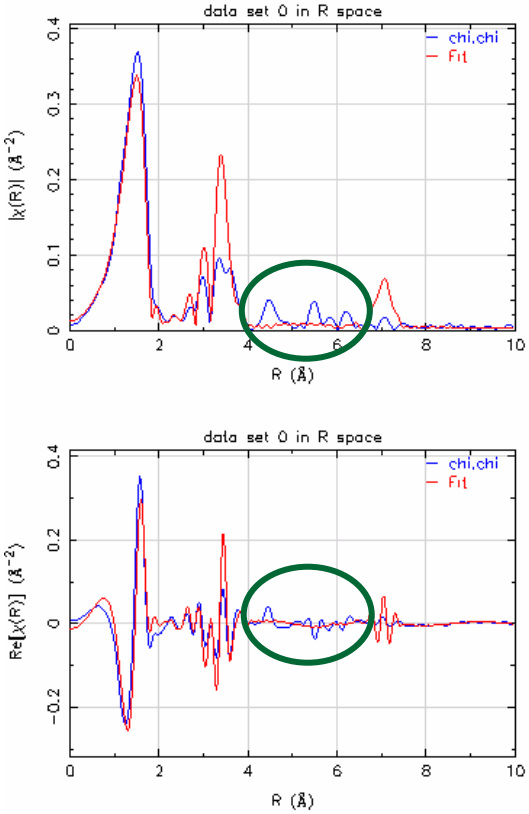
All data is present in model

Minimum amplitude 10%
18 of 69 paths



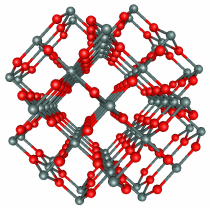
missing a little of the data

Minimum amplitude 15%
8 of 69 paths



missing a lot of the data

Models to consider:

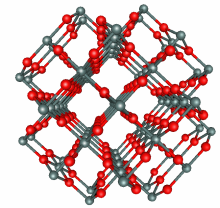


- Δr:
  - Symmetric expansion term: Alpha * reff.
  - Grouped depending on distance and atom types
  - Related to unit cell dimensions
- ΔE:
  - Energy shifts that depend on atom type
  - One energy shift for all paths
  - Two energy shifts, one for first shell and another for all other shells
- σ^2:
  - Grouped depending on distance and atom types.
  - Use a Debye or Einstien 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

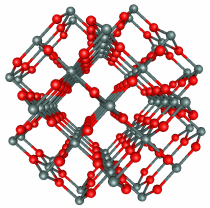
- **Multiple edges, structural information**: B Ravel, E. Cockayne, M. Newville and K. M. Rabe. "Combined EXAFS and first-principles theory study of Pb1-xGexTe." Phys. Rev. B **60**(21): pp 14632–14642, Dec 1999
- **Structural information, bond angles**: A. I. Frenkel, E A Stern, A. Voronel, M. Qian 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(NH2)3]6[(UO2)3(CO3)6] 6.5H20." 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 KNbO3 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 $La_{2-x}Sr_xCuO_4$" 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 BaTiO3." 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.

The Model for SnO_2 data

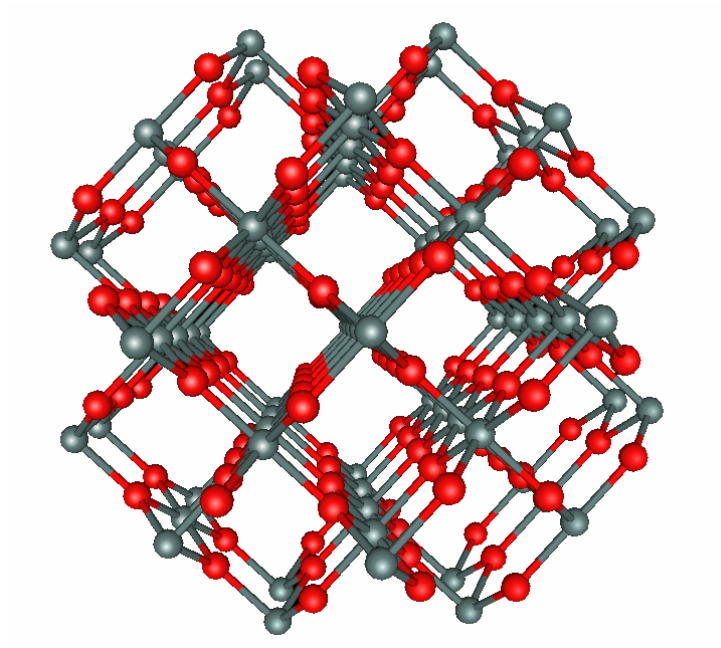


- Δr: symmetric expansion term: Alpha * reff.
- ΔE: Energy shifts that depend on atom type:
  - The first shell; Eo1,
  - All other oxygen scattering events: Eo2
  - All tin scattering events: Esn
- σ^2: Grouped depending on distance and atom types.
- S02: one for all paths.
- N: determined from the crystal structure.

Final Model for SnO_2



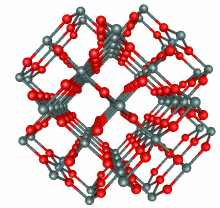
Includes all the atoms shown here

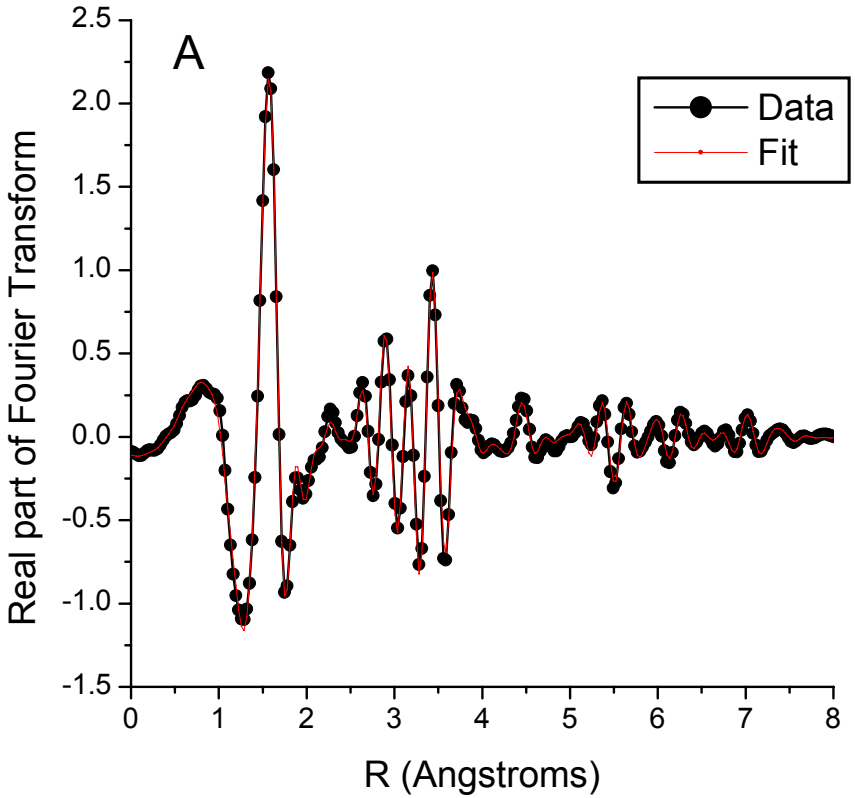


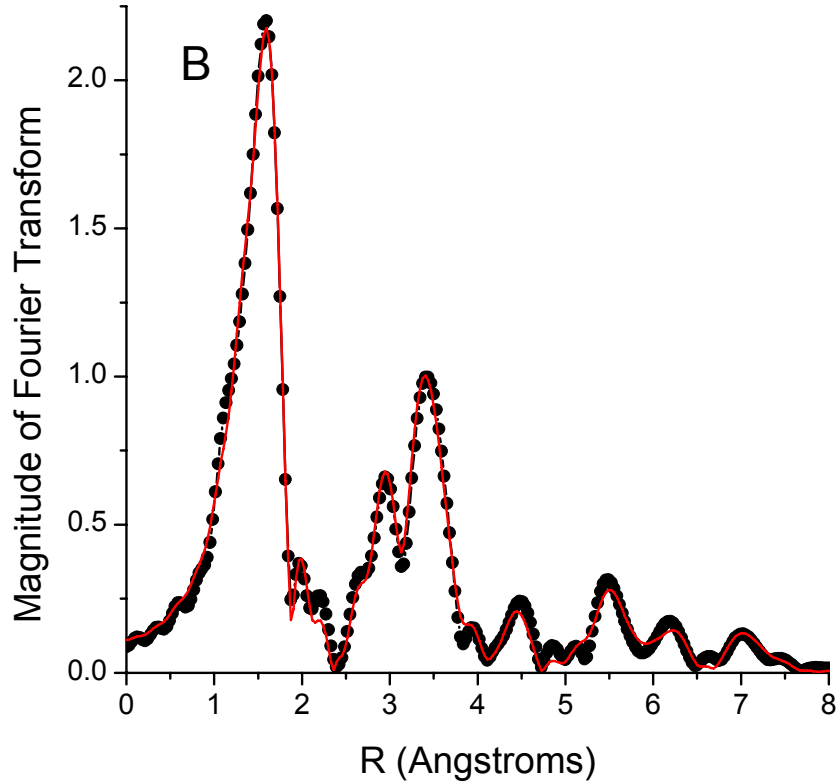
Path	*N*	*reff*	*ΔR*	σ^2	*ΔE*
Sn-O1	4	2.0519	**Alpha**·reff	**σ^2o1**	**ΔEo1**
Sn-O2	2	2.0567	Alpha·reff	σ^2o1	ΔEo1
Sn-Sn1	2	3.1864	Alpha·reff	**σ^2sn1**	**ΔEsn**
Sn-O3	4	3.5906	Alpha·reff	**σ^2o3**	**ΔEo2**
Sn-Sn2	8	3.7093	Alpha·reff	**σ^2sn2**	ΔEsn
Sn-Sn2-01	8	3.9090	Alpha·reff	**σ^2sn2o1**	0.5·ΔEsn+0.5·ΔEo1
Sn-Sn2-02	8	3.9090	Alpha·reff	σ^2sn2o1	0.5·ΔEsn+0.5·ΔEo1
Sn-O5	8	4.2414	Alpha·reff	**σ^2o5**	ΔEo2
Sn-Sn3	4	4.7373	Alpha·reff	**σ^2sn3**	ΔEsn
Sn-O7	8	4.8006	Alpha·reff	**σ^2o7**	ΔEo2
Sn-Sn4	8	5.7092	Alpha·reff	**σ^2sn4**	ΔEsn
Sn-Sn5	8	5.8365	Alpha·reff	σ^2sn4	ΔEsn
Sn-Sn5-01	8	5.8405	Alpha·reff	σ^2sn4	0.5·ΔEsn+0.5·ΔEo1
Sn-Sn5-04	8	5.8405	Alpha·reff	σ^2sn4	0.5·ΔEsn+0.5·ΔEo2
Sn-O1-Sn5-O1	4	5.8444	Alpha·reff	σ^2sn4	0.33·ΔEsn+0.66·ΔEo1
Sn-O4-Sn5-O4	4	5.8444	Alpha·reff	σ^2sn4	0.33·ΔEsn+0.66·ΔEo2
Sn-Sn6-Sn1	4	6.3728	Alpha·reff	**σ^2sn6**	ΔEsn
Sn-Sn1-Sn6-Sn1	2	6.3728	Alpha·reff	σ^2sn6	ΔEsn
Sn-Sn7	4	6.6995	Alpha·reff	**σ^2sn7**	ΔEsn
Sn-Sn7-O2	4	6.6995	Alpha·reff	σ^2sn7	0.5·ΔEsn+0.5·ΔEo1
Sn-Sn7-O6	4	6.6995	Alpha·reff	σ^2sn7	0.5·ΔEsn+0.5·ΔEo2
Sn-Sn7-O6-O2	4	6.6995	Alpha·reff	σ^2sn7	0.33·ΔEsn+0.33·ΔEo1+0.33·ΔEo2
Sn-O6-Sn7-O2	4	6.6995	Alpha·reff	σ^2sn7	0.33·ΔEsn+0.33·ΔEo1+0.33·ΔEo2
Sn-O2-Sn7-O6-O2	4	6.6995	Alpha·reff	σ^2sn7	0.25·ΔEsn+0.50·ΔEo1+0.25·ΔEo2
Sn-O6-Sn7-O6-O2	4	6.6995	Alpha·reff	σ^2sn7	0.25·ΔEsn+0.25·ΔEo1+0.50·ΔEo2
Sn-Sn8	8	7.4187	Alpha·reff	**σ^2sn8**	ΔEsn
Sn-Sn8-Sn2	16	7.4187	Alpha·reff	σ^2sn8	ΔEsn
Sn-Sn2-Sn-Sn2	8	7.4187	Alpha·reff	4·σ^2sn2	ΔEsn
Sn-Sn2-Sn8-Sn2	8	7.4187	Alpha·reff	σ^2sn8	ΔEsn
Sn-Sn9	16	7.6578	Alpha·reff	**σ^2sn9**	ΔEsn

- 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.

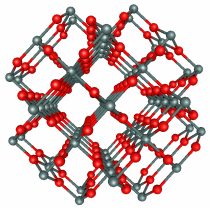
Final Model and Fit to SnO_2





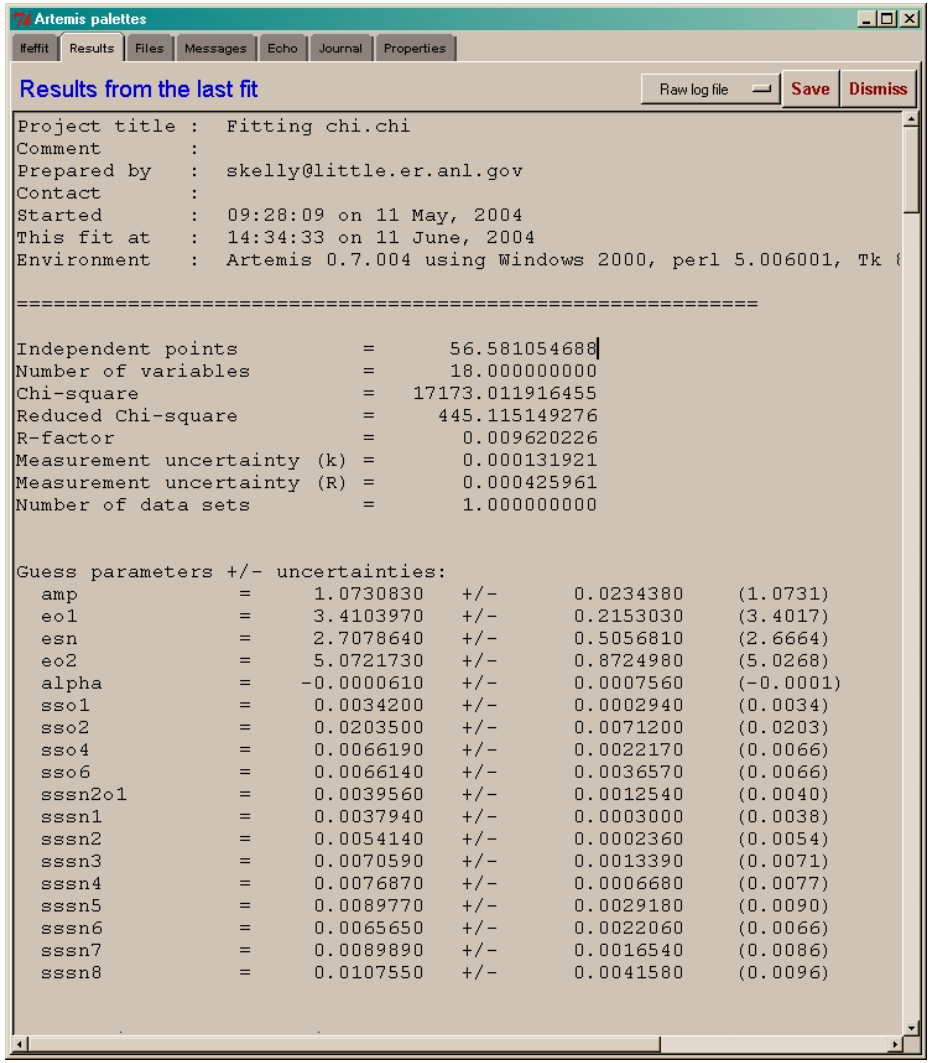


Evaluating fit Results



Typical values for EXAFS parameters

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



Artemis palettes

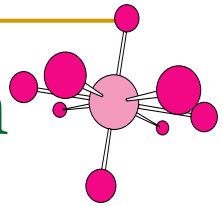
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit

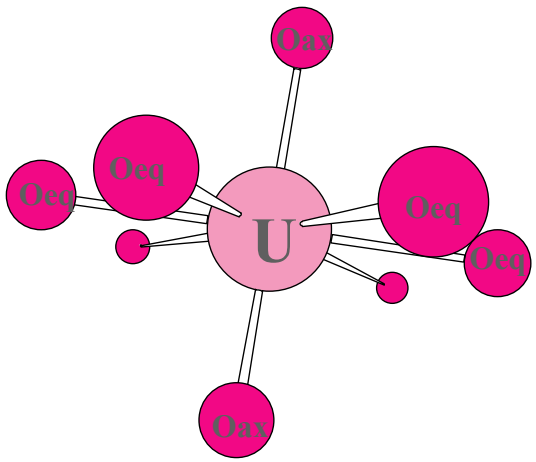
Raw log file | Save | Dismiss

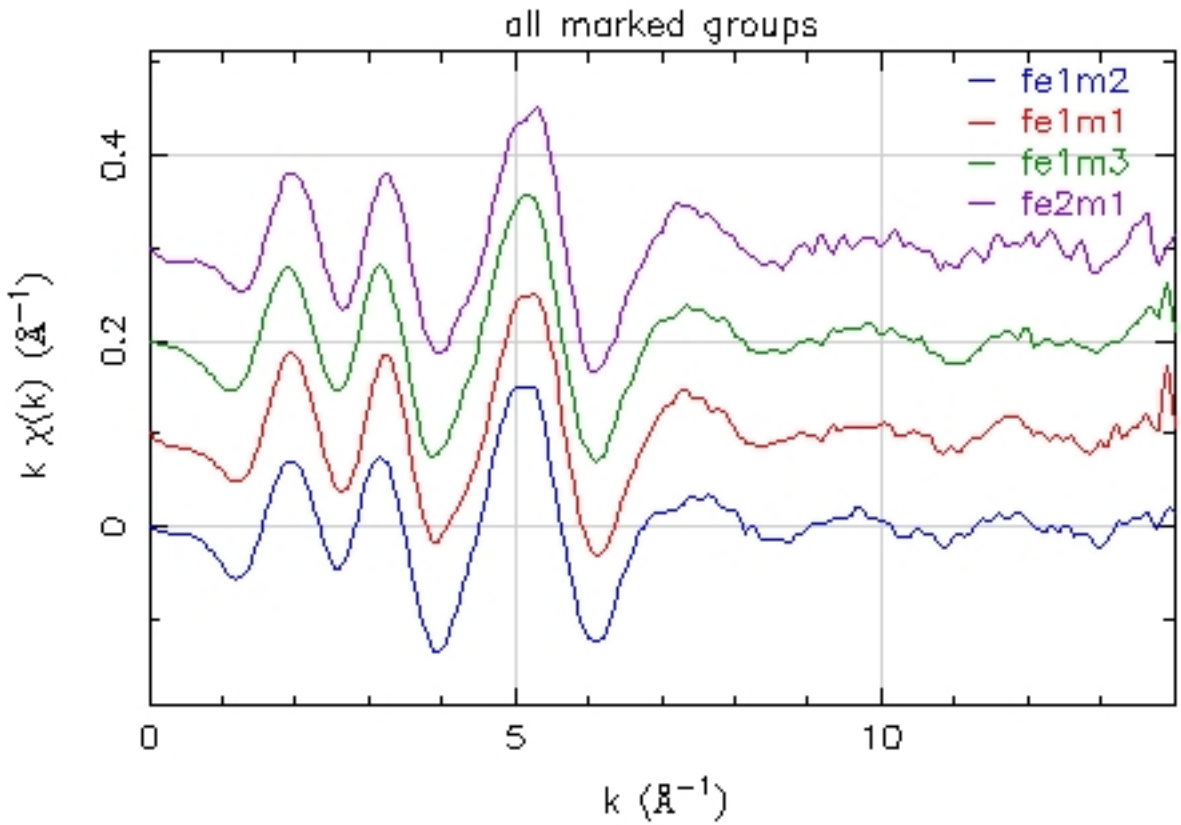
```
Project title :  Fitting chi.chi
Comment       :
Prepared by   :  skelly@little.er.anl.gov
Contact       :
Started       :  09:28:09 on 11 May, 2004
This fit at   :  14:34:33 on 11 June, 2004
Environment   :  Artemis 0.7.004 using Windows 2000, perl 5.006001, Tk 8

==============================================================

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

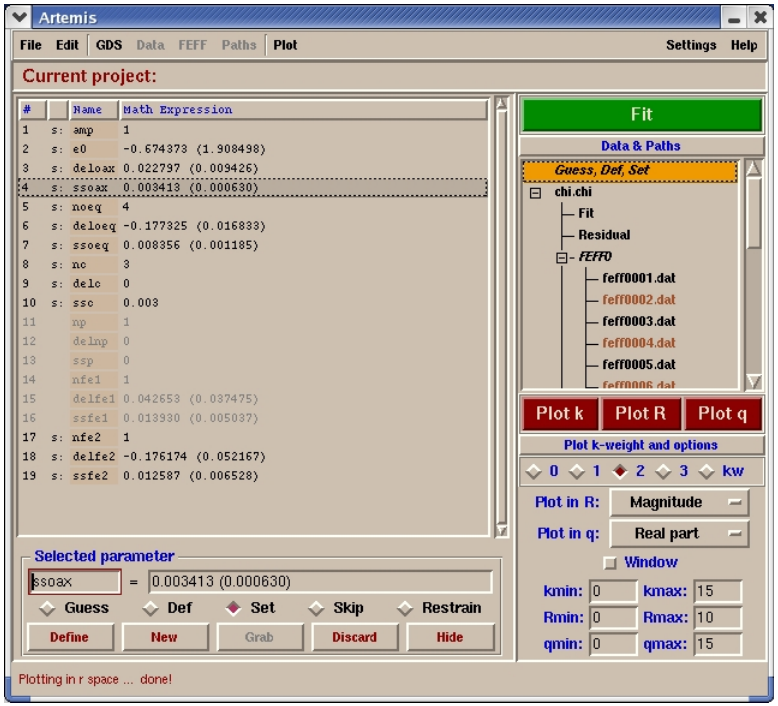


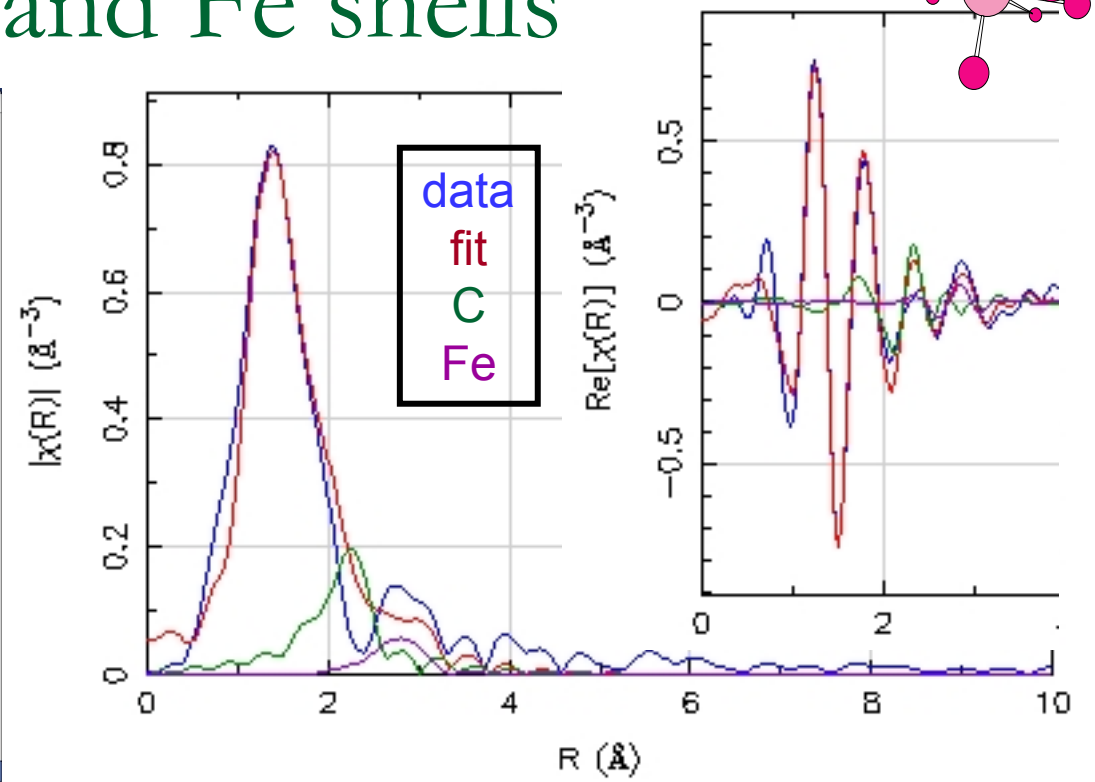
- Uranyl in equilibrium with a mixture of Fe-oxides and different microbial components.
- Possible second shell atoms, O, C, P, Fe, U.
- 30-50 combinations of these atoms were tested.
- Three of these tests are shown here:
  - C and Fe,
  - P and Fe,
  - Fe and Fe

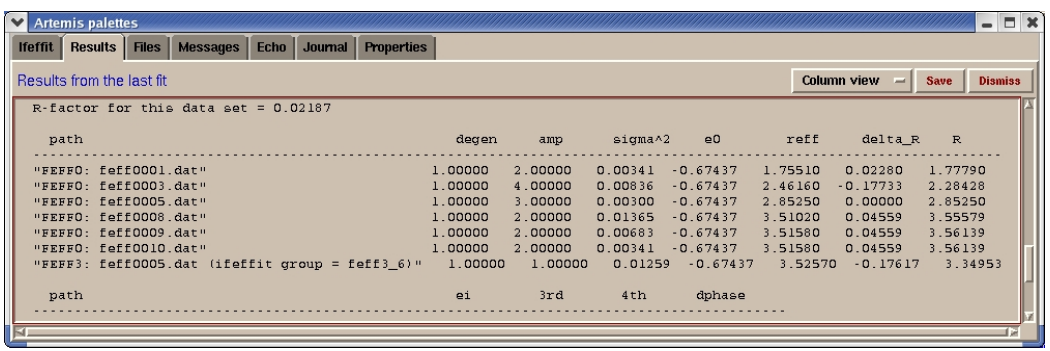




Test data for C and Fe shells



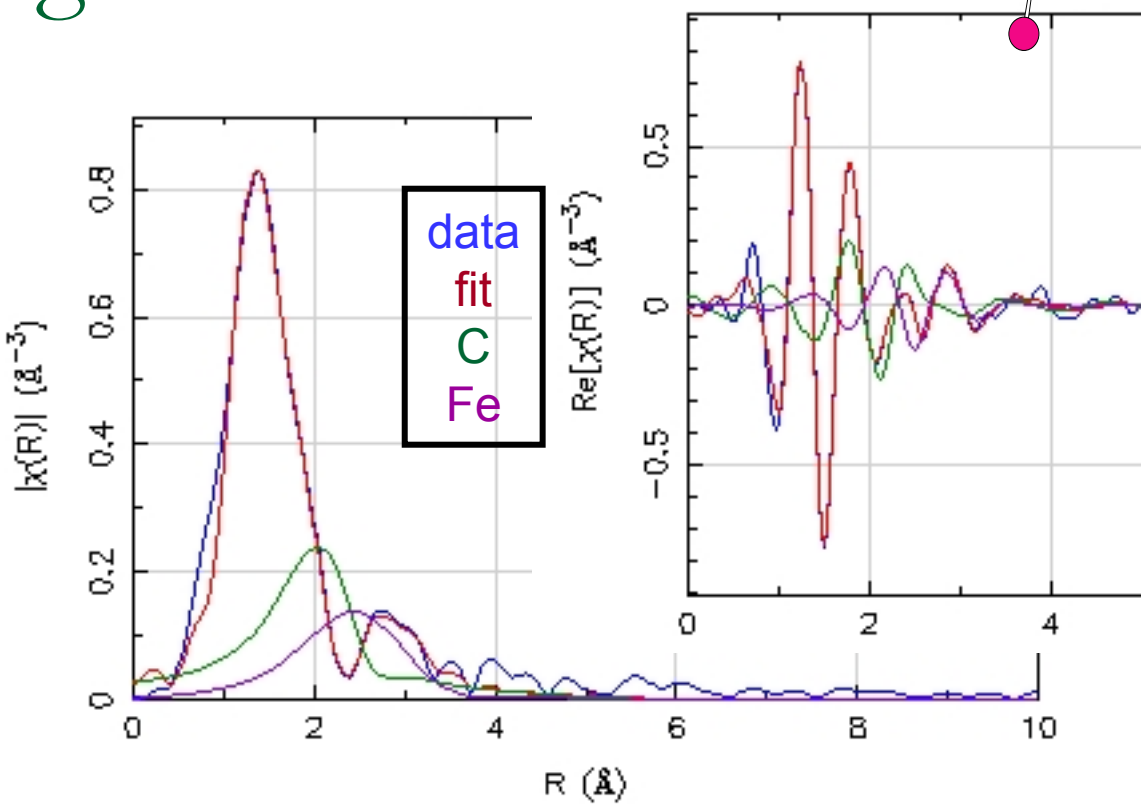


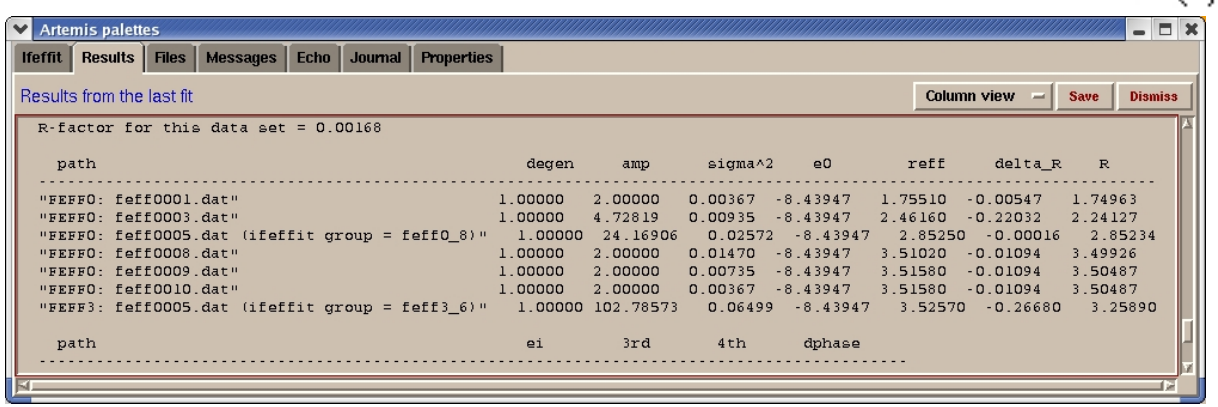


- Place **C** and **Fe** shells in a "good" spot
  - set parameters – no fitting
  - monitor results and fit spectra

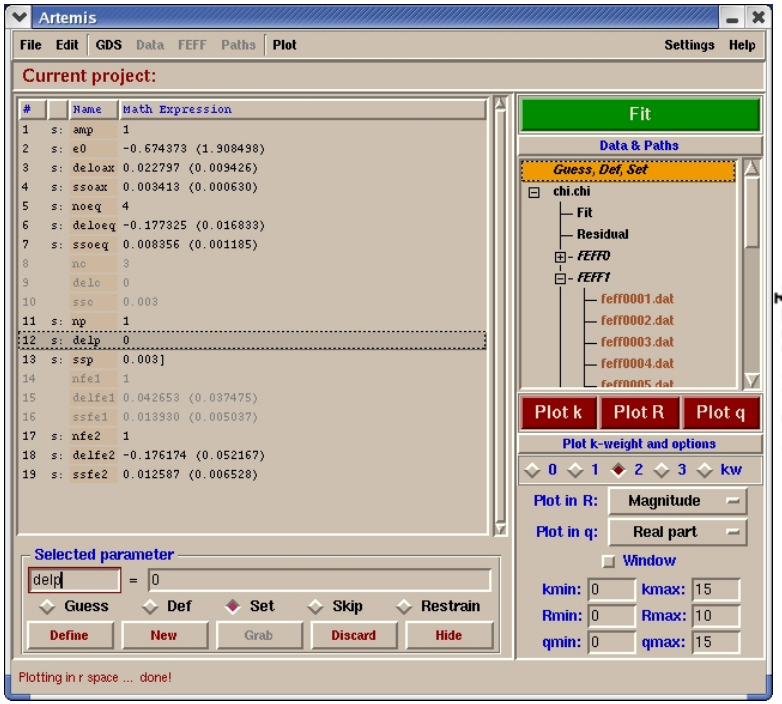
Fit Results using C and Fe shells

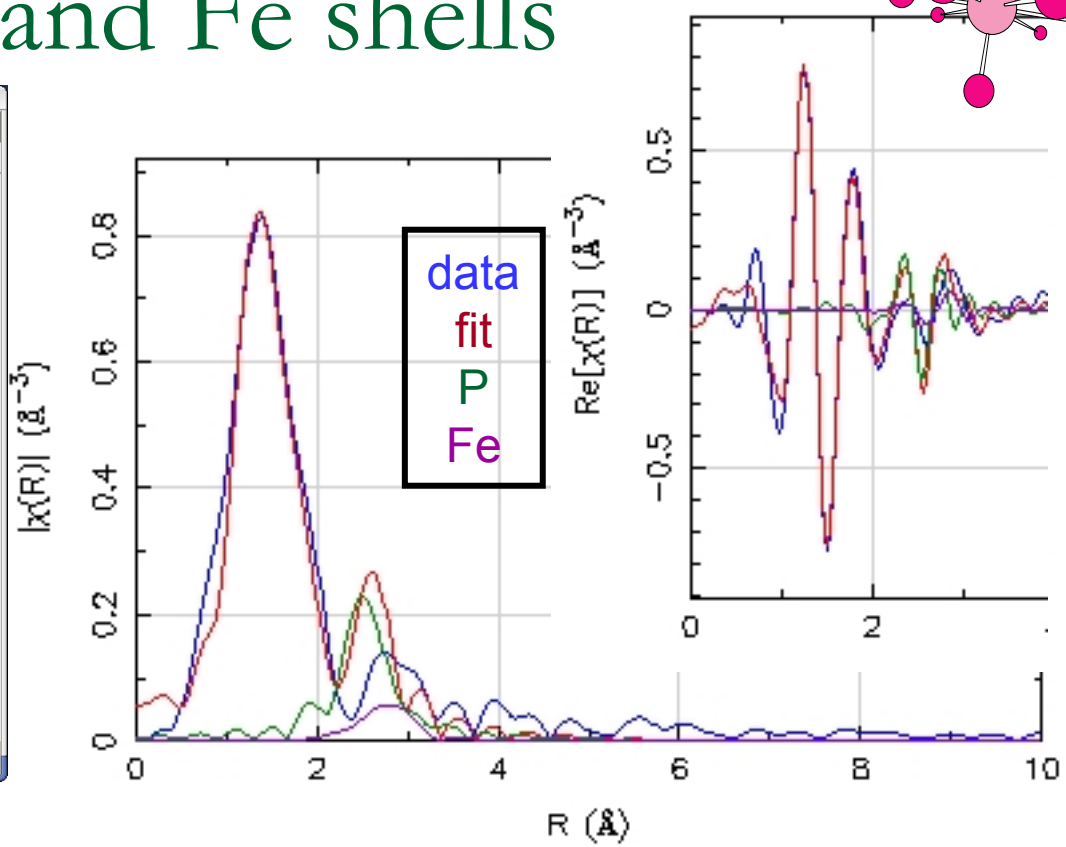
EXAFS Parameters	
σ^2-values	-
Distances	+
Coordination numbers	-
ΔE-value	-

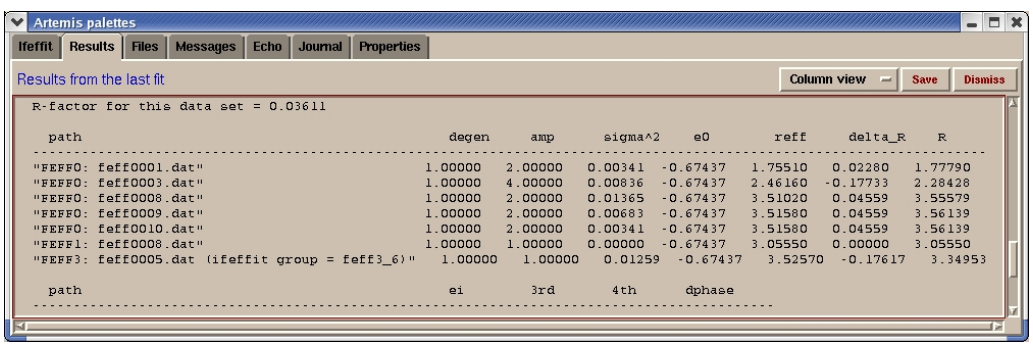




Test data for P and Fe shells



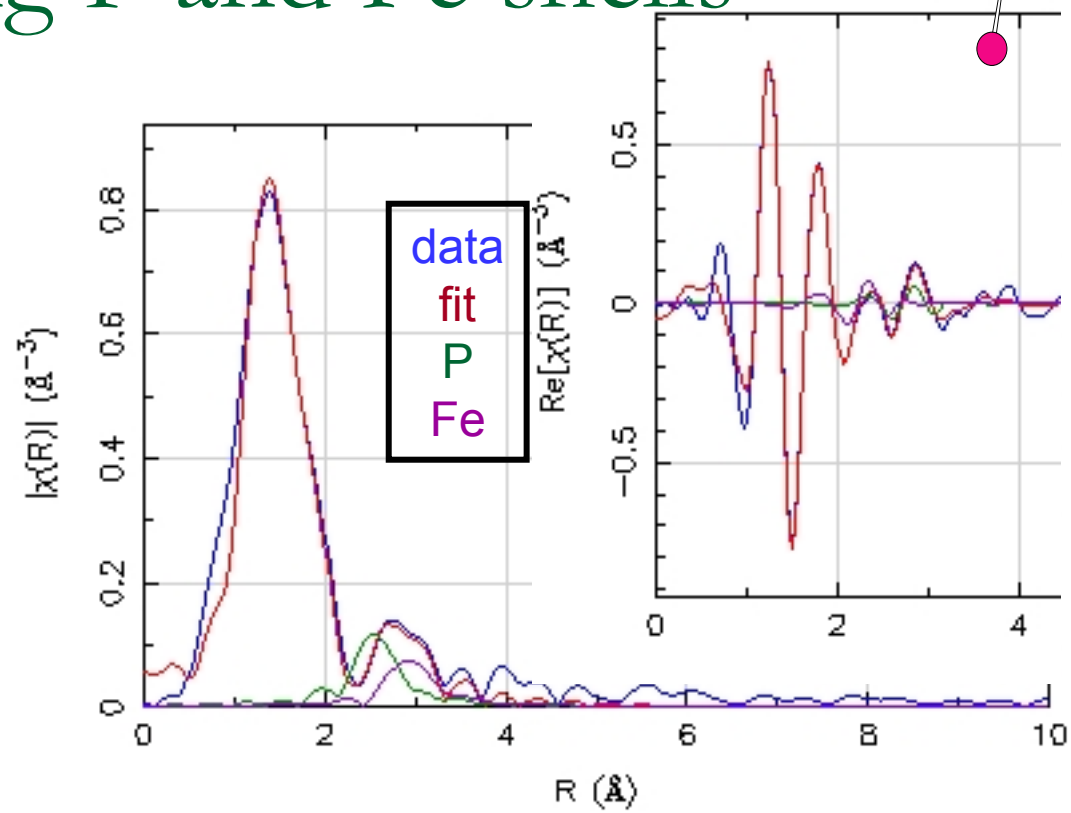


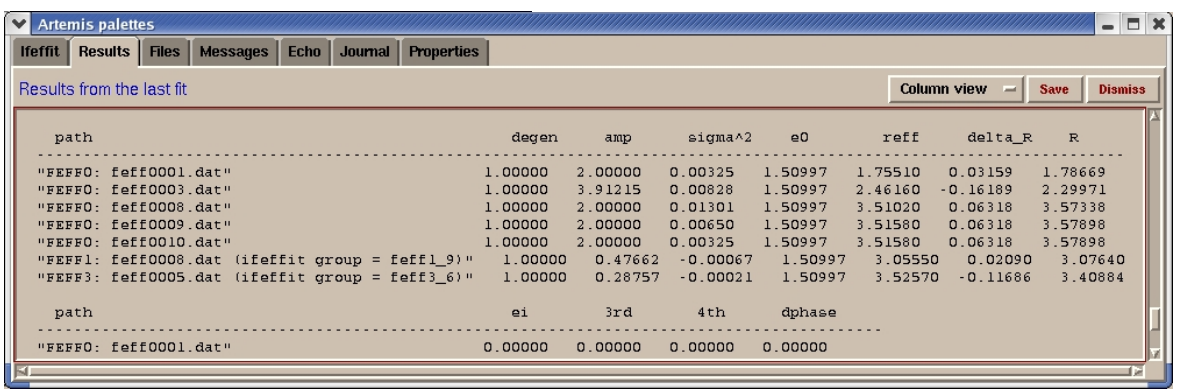


- Place **P** and **Fe** shells in a "good" spot
  - set parameters – no fitting
  - monitor results and fit spectra

Fit Results using P and Fe shells

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





Artemis palettes

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

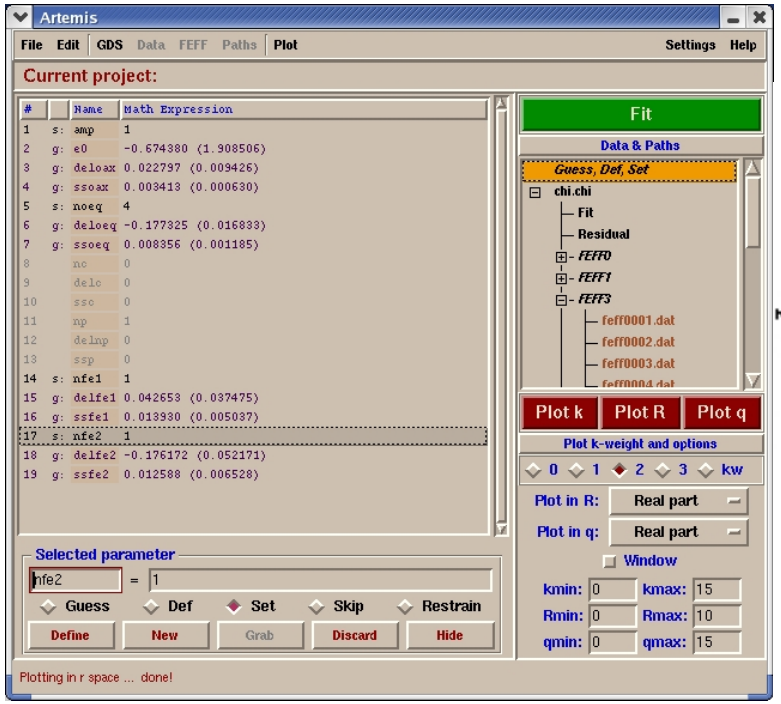
Results from the last fit

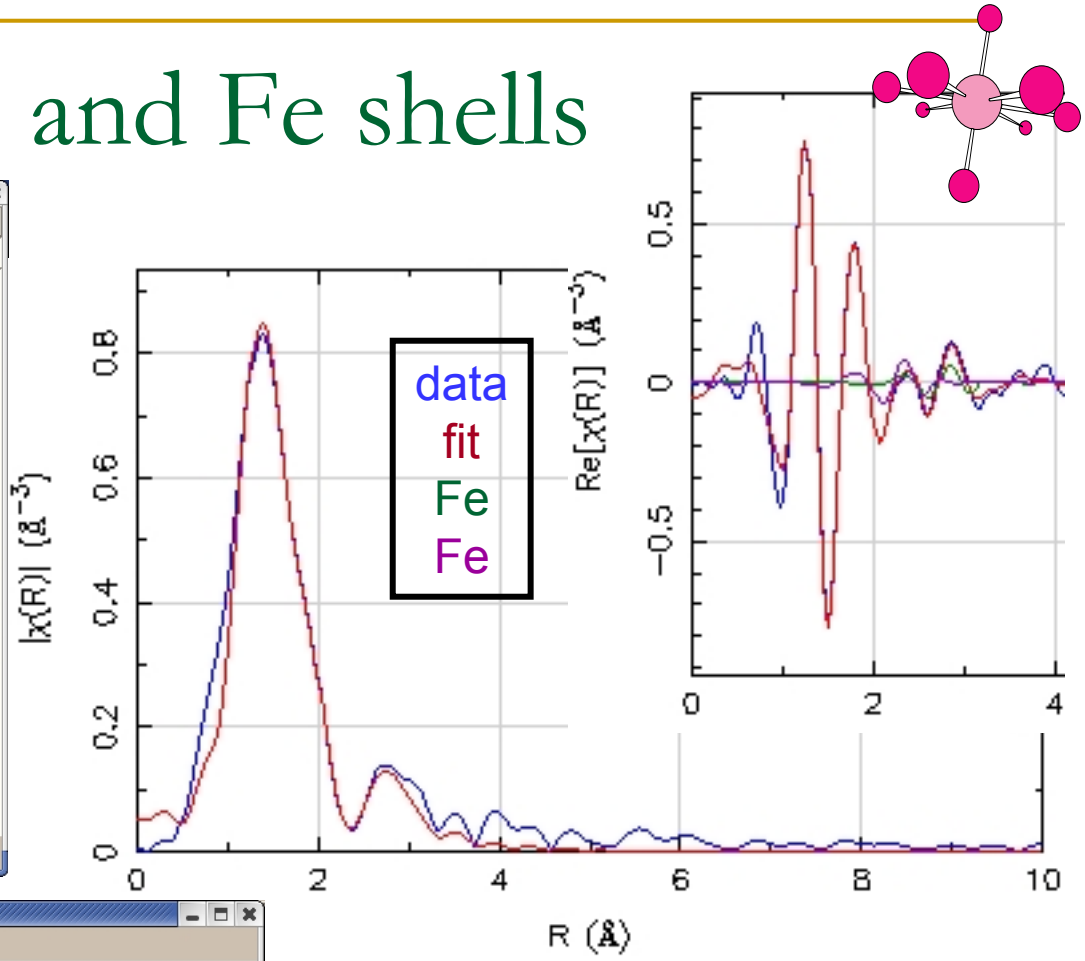
Column view | Save | Dismiss

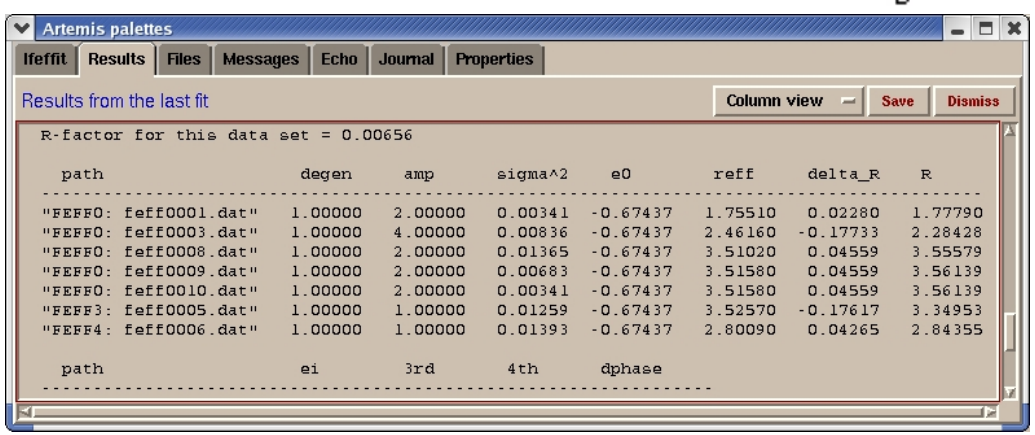
path	degen	amp	sigma^2	e0	reff	delta_R	R
"FEFF0: feff0001.dat"	1.00000	2.00000	0.00325	1.50997	1.75510	0.03159	1.78669
"FEFF0: feff0003.dat"	1.00000	3.91215	0.00828	1.50997	2.46160	-0.16189	2.29971
"FEFF0: feff0008.dat"	1.00000	2.00000	0.01301	1.50997	3.51020	0.06318	3.57338
"FEFF0: feff0009.dat"	1.00000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

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

Test data for Fe and Fe shells



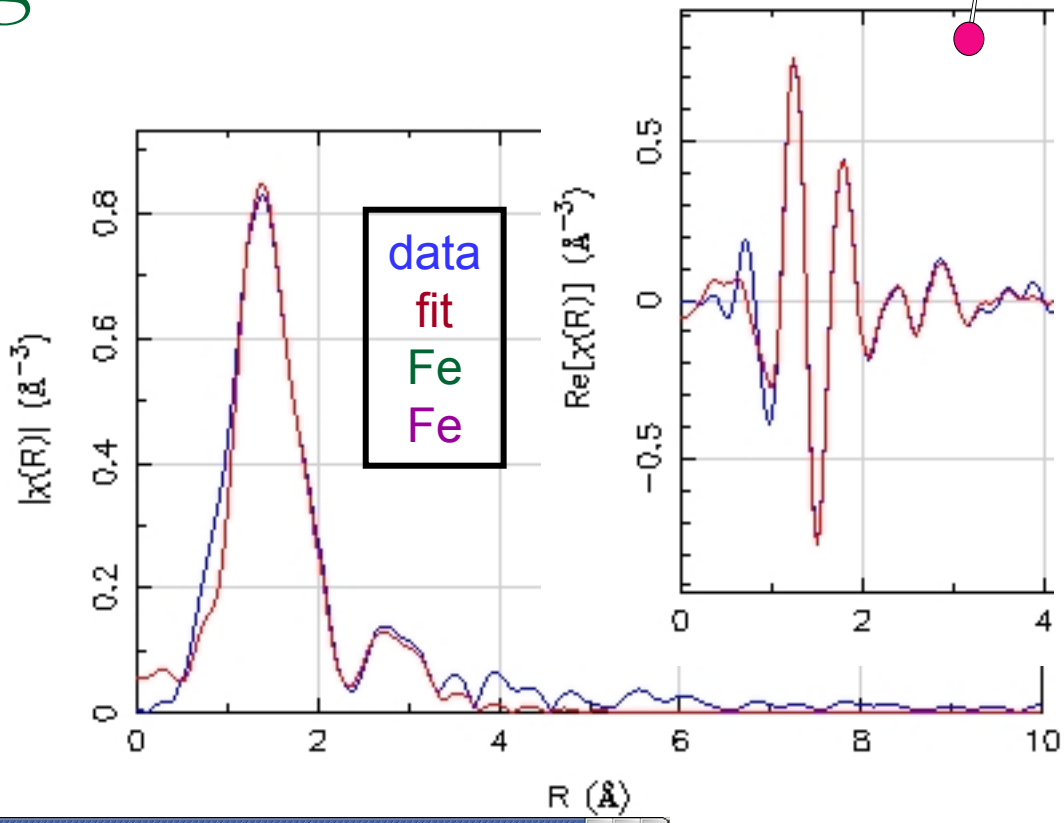


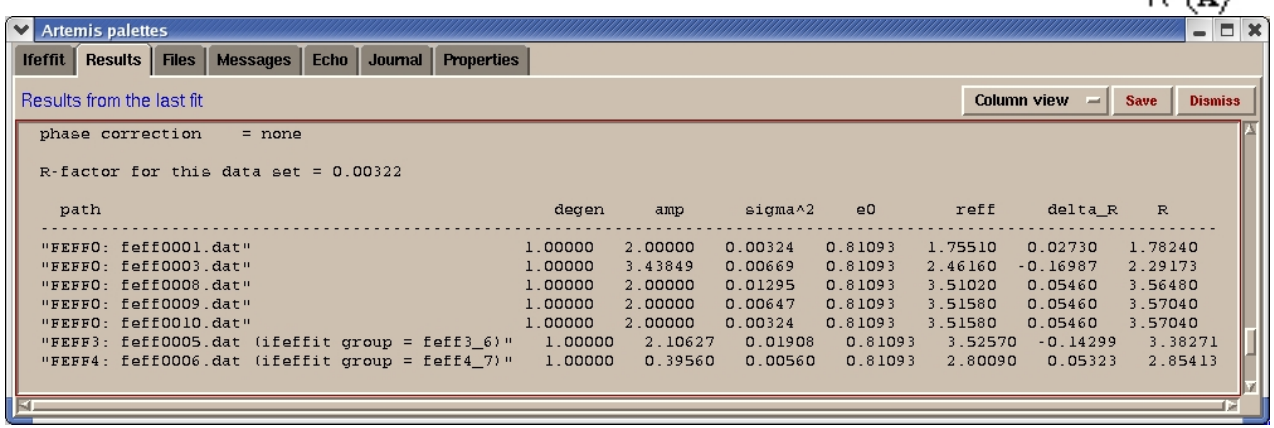


- Place Fe and Fe shells in a “good” spot
  - set parameters – no fitting
  - monitor results and fit spectra

Fit Results using Fe and Fe shells

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

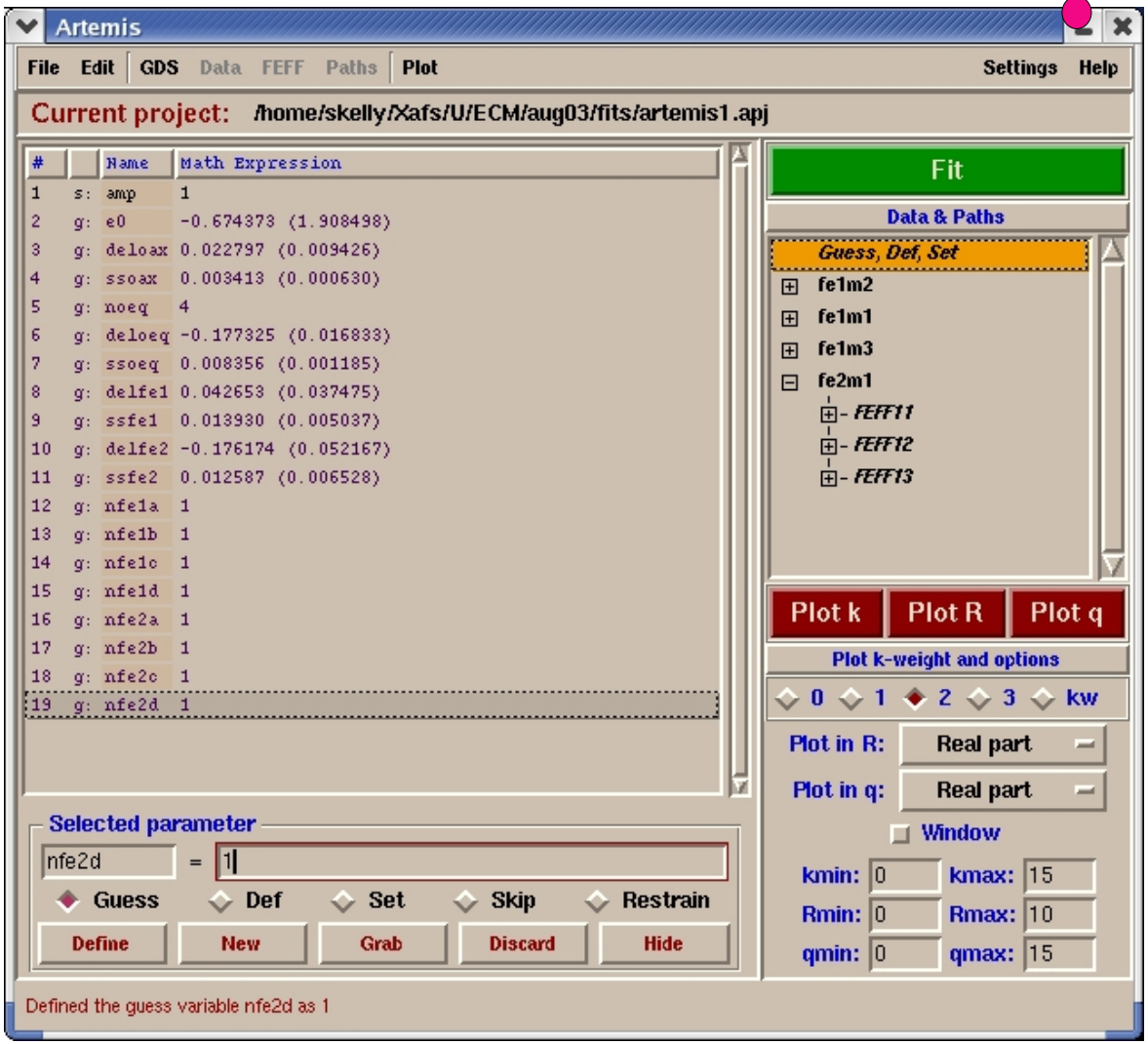




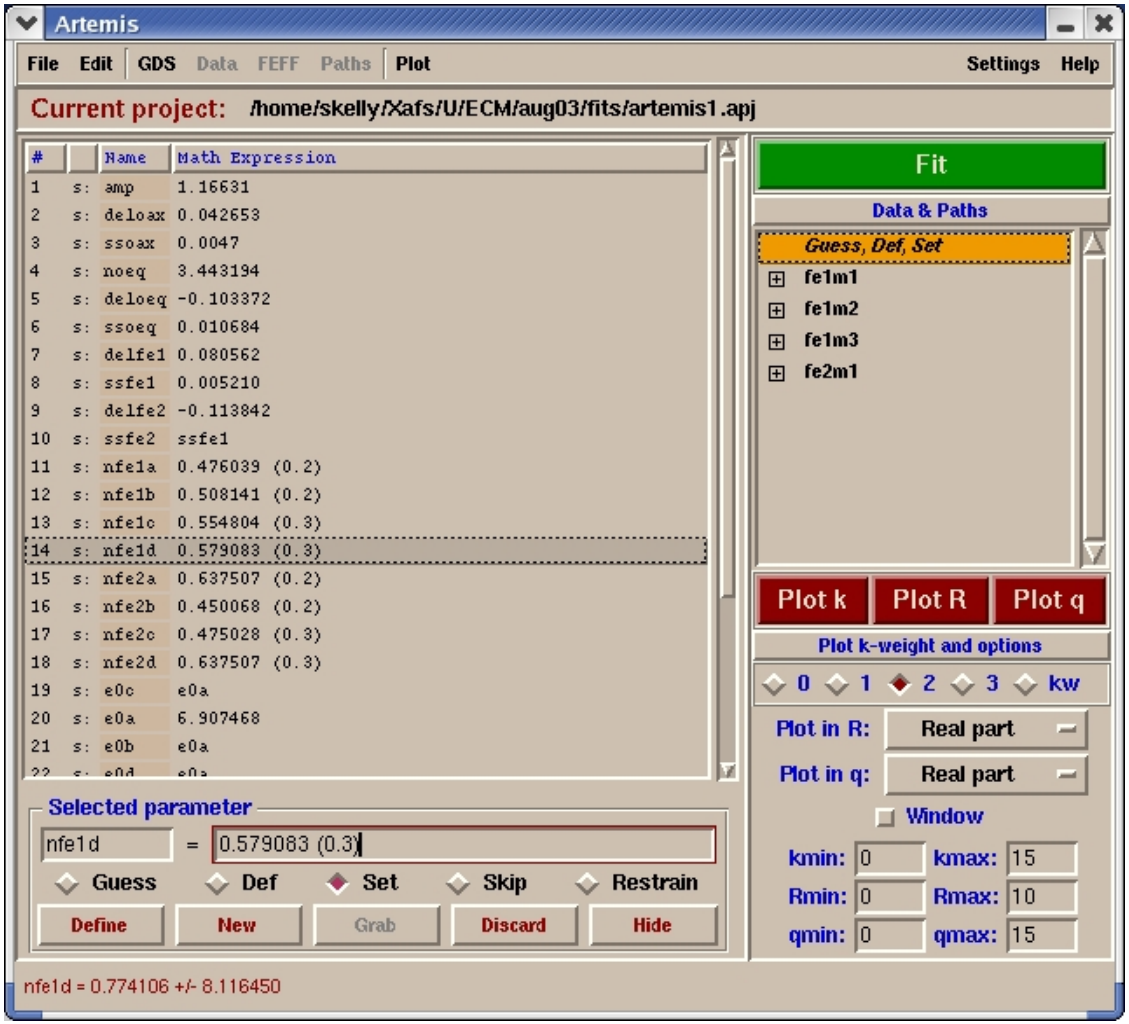

```
phase correction     = none

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

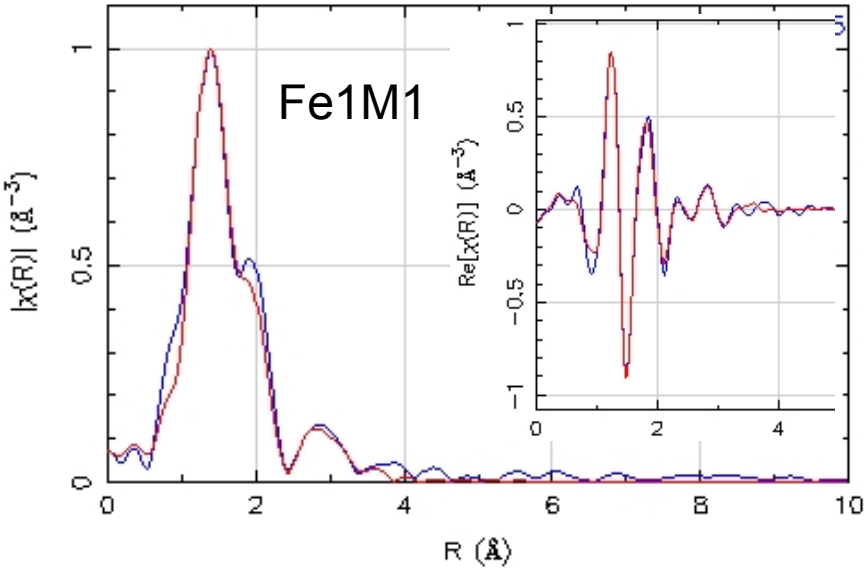


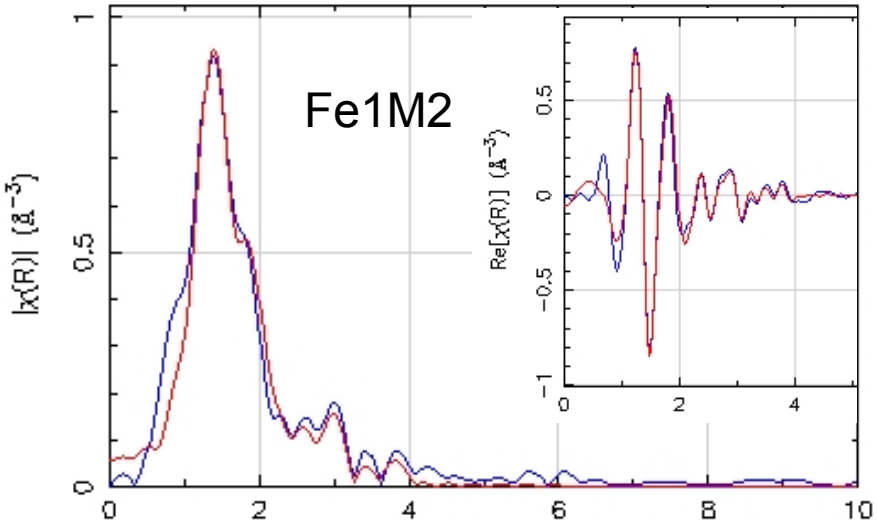
Modeling a Data Series

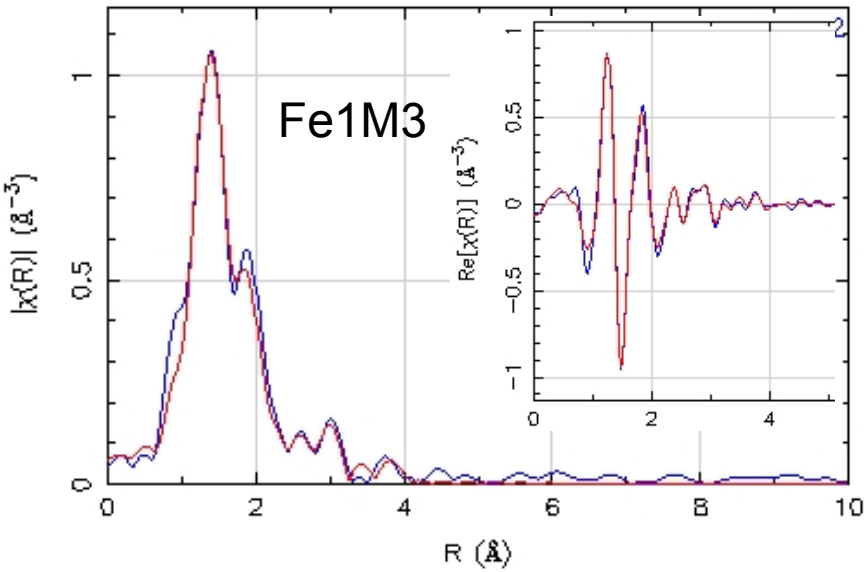


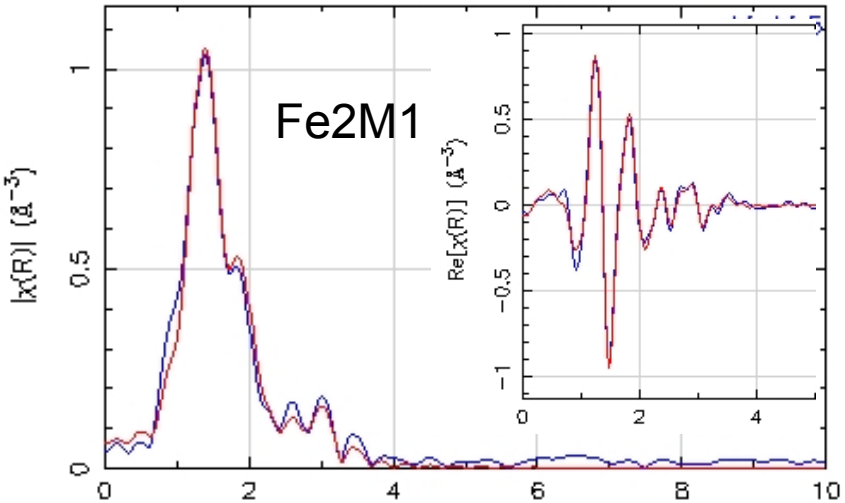
- Coordination number is determined within 5%
- Assuming model is accurate!

Fit results from data series

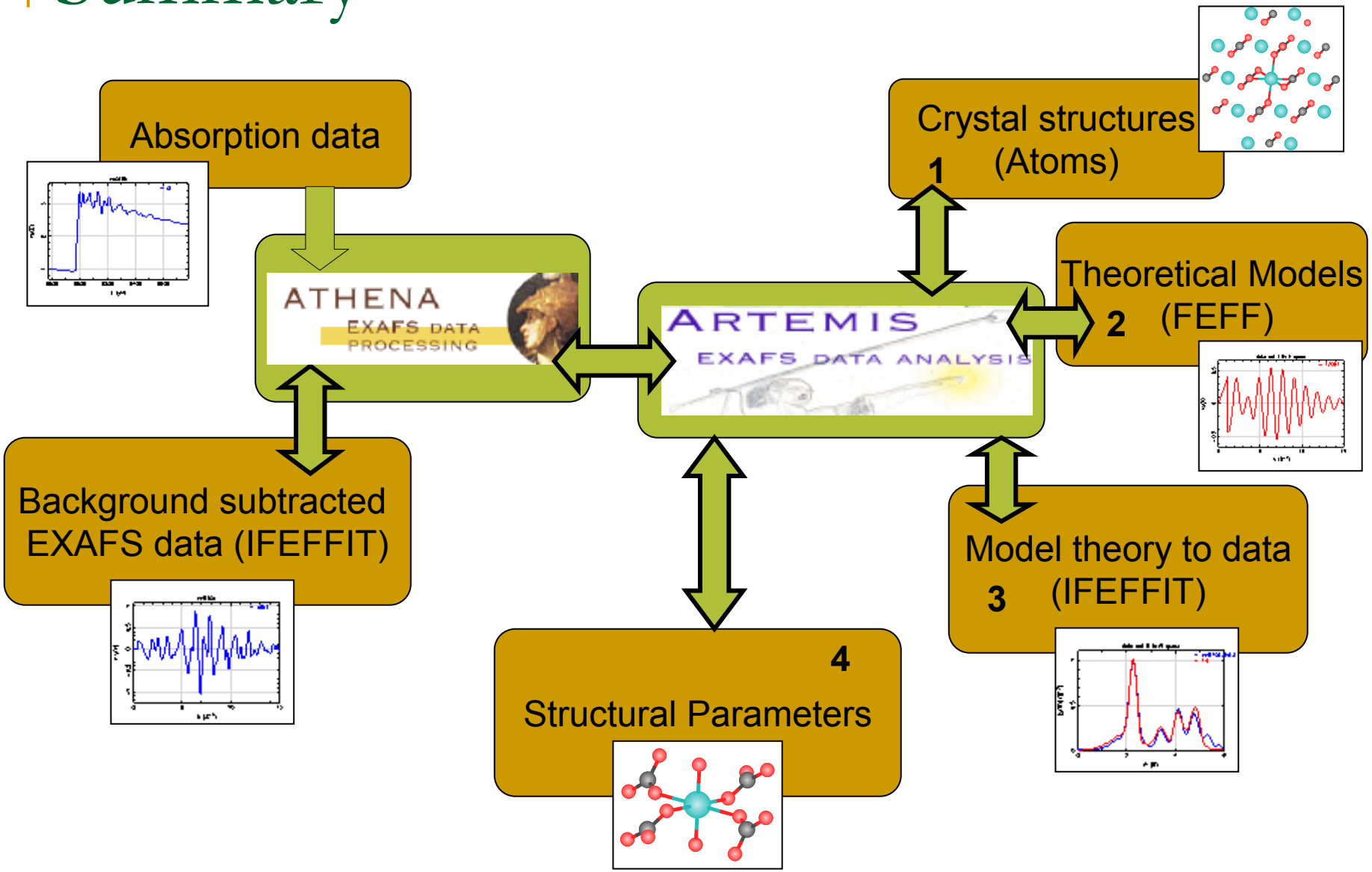








Summary


Absorption data
ATHENA
EXAFS DATA PROCESSING
ARTEMIS
EXAFS DATA ANALYSIS
Crystal structures
1
(Atoms)
Theoretical Models
2
(FEFF)
Background subtracted
EXAFS data (IFEFFIT)
Model theory to data
3
(IFEFFIT)
4
Structural Parameters