X-ray Absorption Fine Structure Overview

Shelly D. Kelly

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X-rays and Matter

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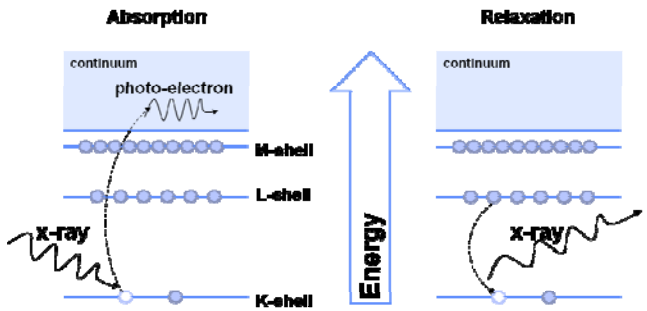
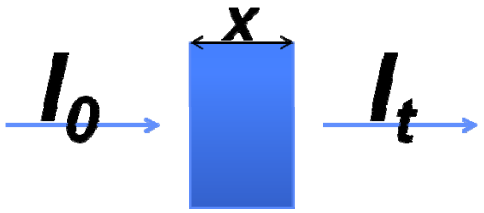
- **Photoelectric effect (Einstein's 1921 Nobel Prize):**
  - **Dominates for X-rays with energies from 500 eV to 500 keV**
  - **X-ray photon is absorbed by an electron in a tightly bound quantum core level of an atom.**
  - **Binding energy of electron must be less than x-ray energy otherwise the electron does not interact with the X-ray.**
  - **The x-ray is destroyed (absorbed) and excess energy is given to the phot-electron that is ejected from the atom.**

Electronic transitions due to X-ray absorption must follow dipole selection rule requires conservation of angular momentum. Transitions are allow for ℓ = +/- 1

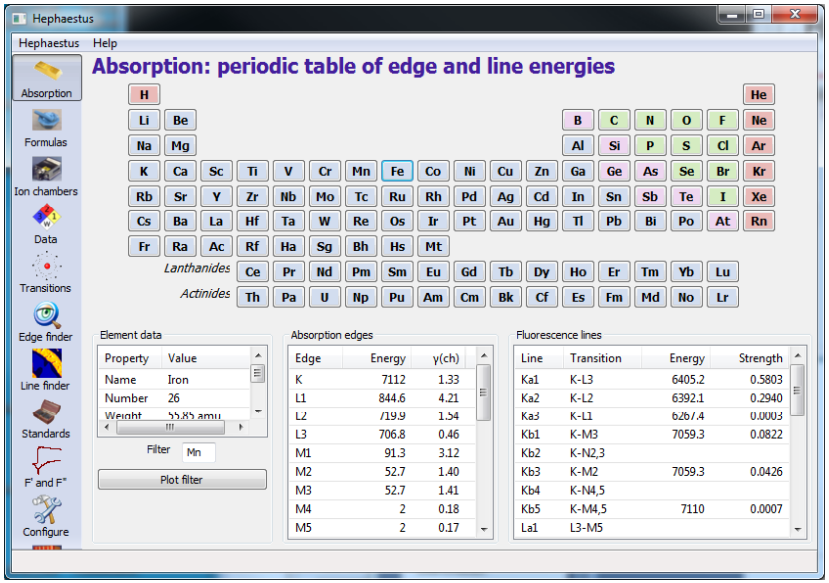


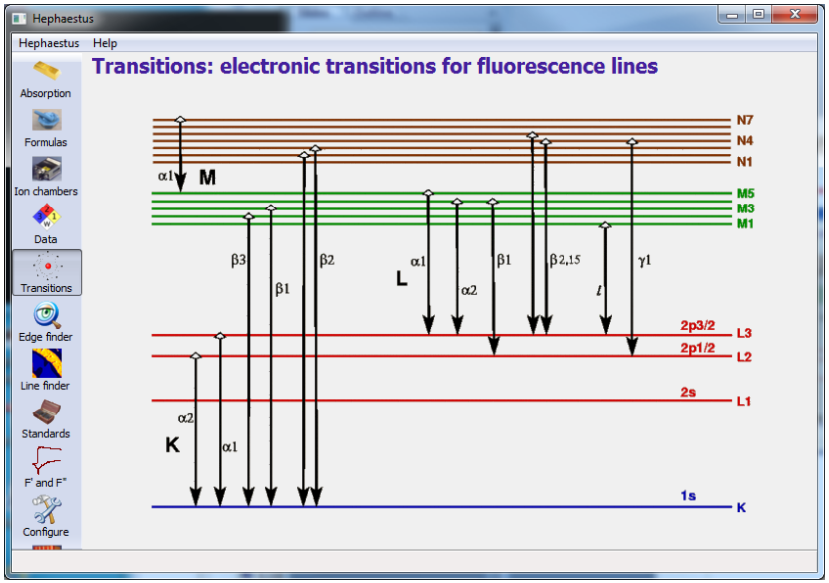
Beer's Law: Absorption of X-rays by Matter

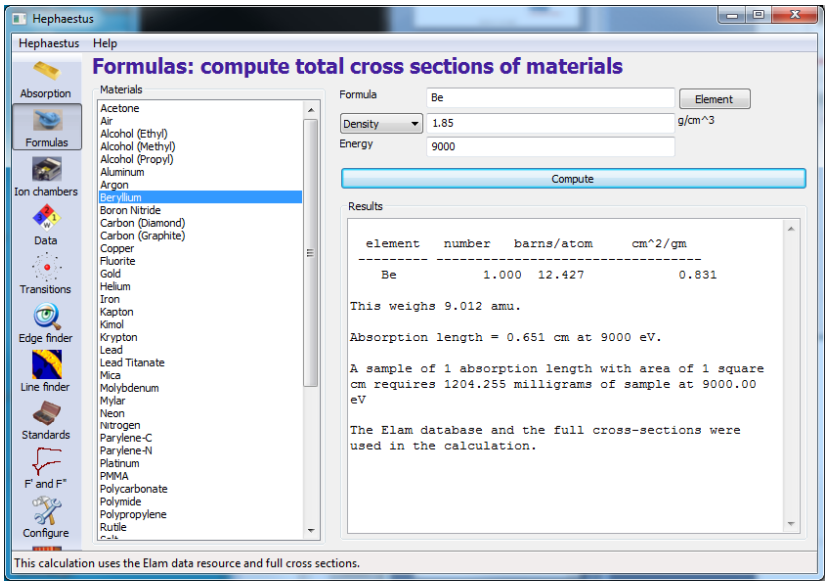
$$I_t = I_0 e^{-\mu x}$$

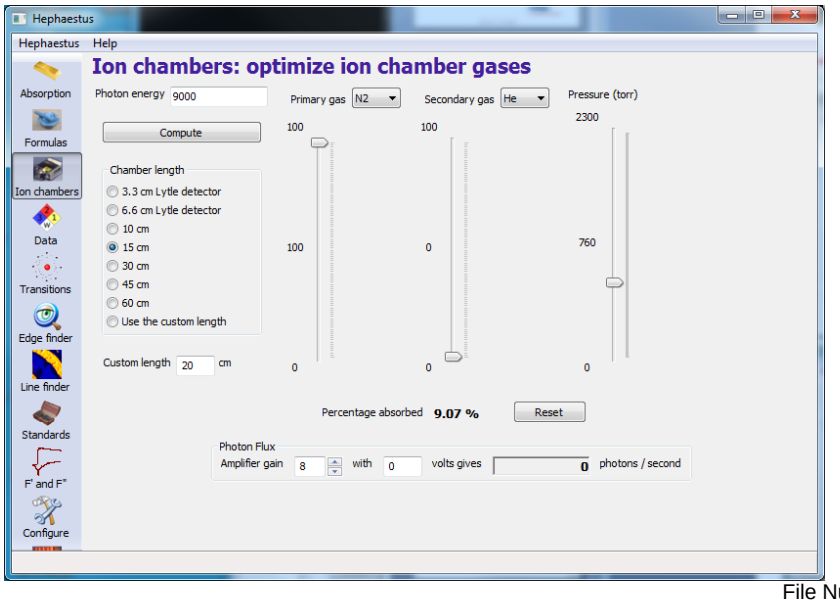


Hephaestus: Absorption Tools









File Number

Measurement of X-ray Absorption Coefficient

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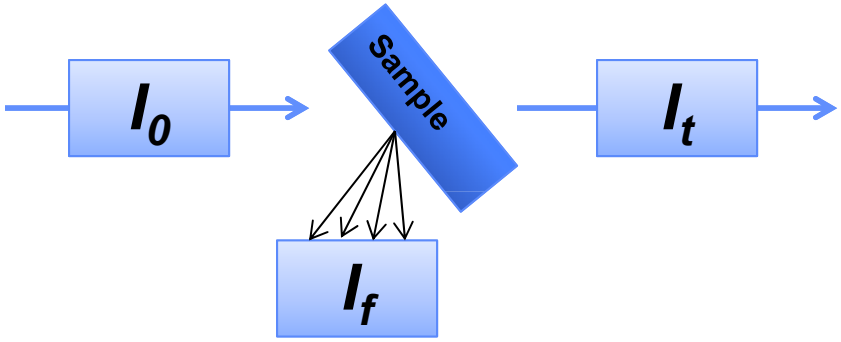
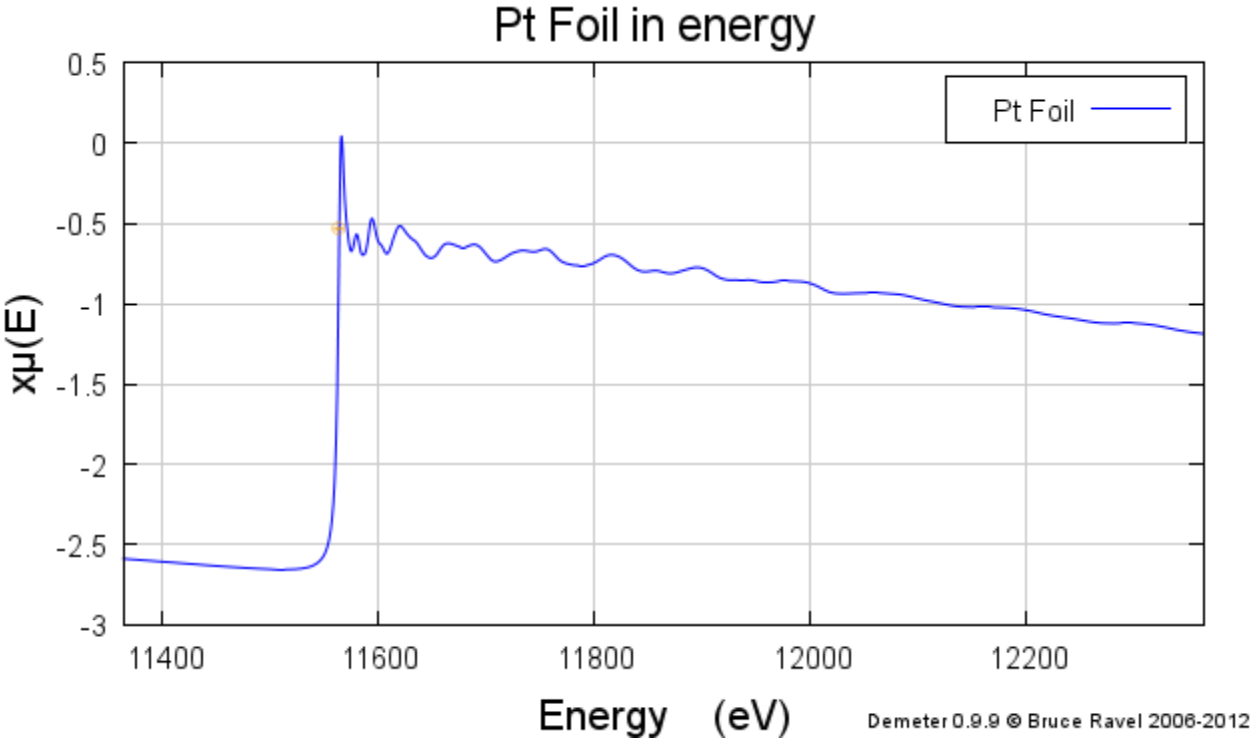
Transmission

$$\mu = \log \frac{I_0}{I_t}$$

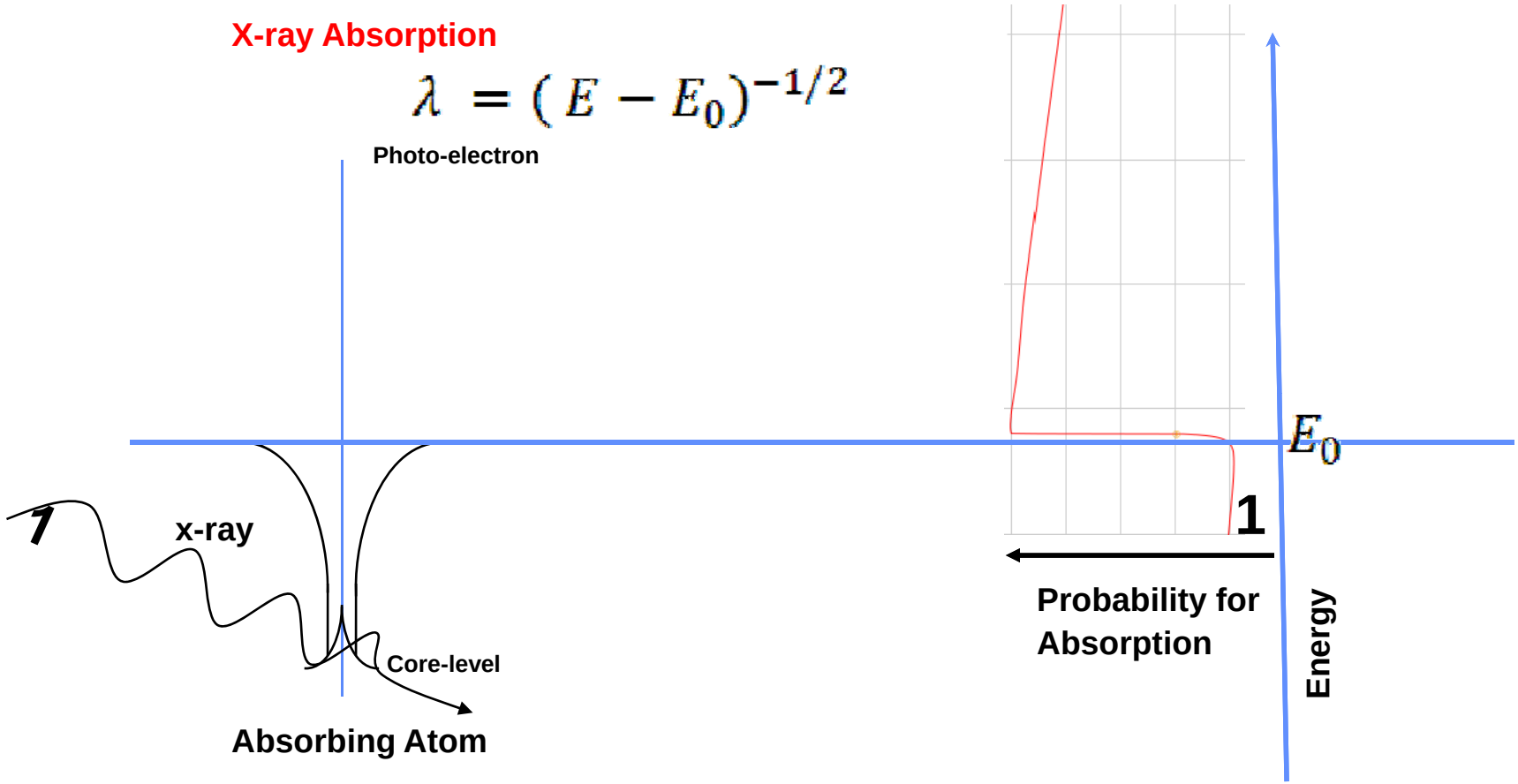


Fluorescence

$$\mu \propto \frac{I_f}{I_0}$$



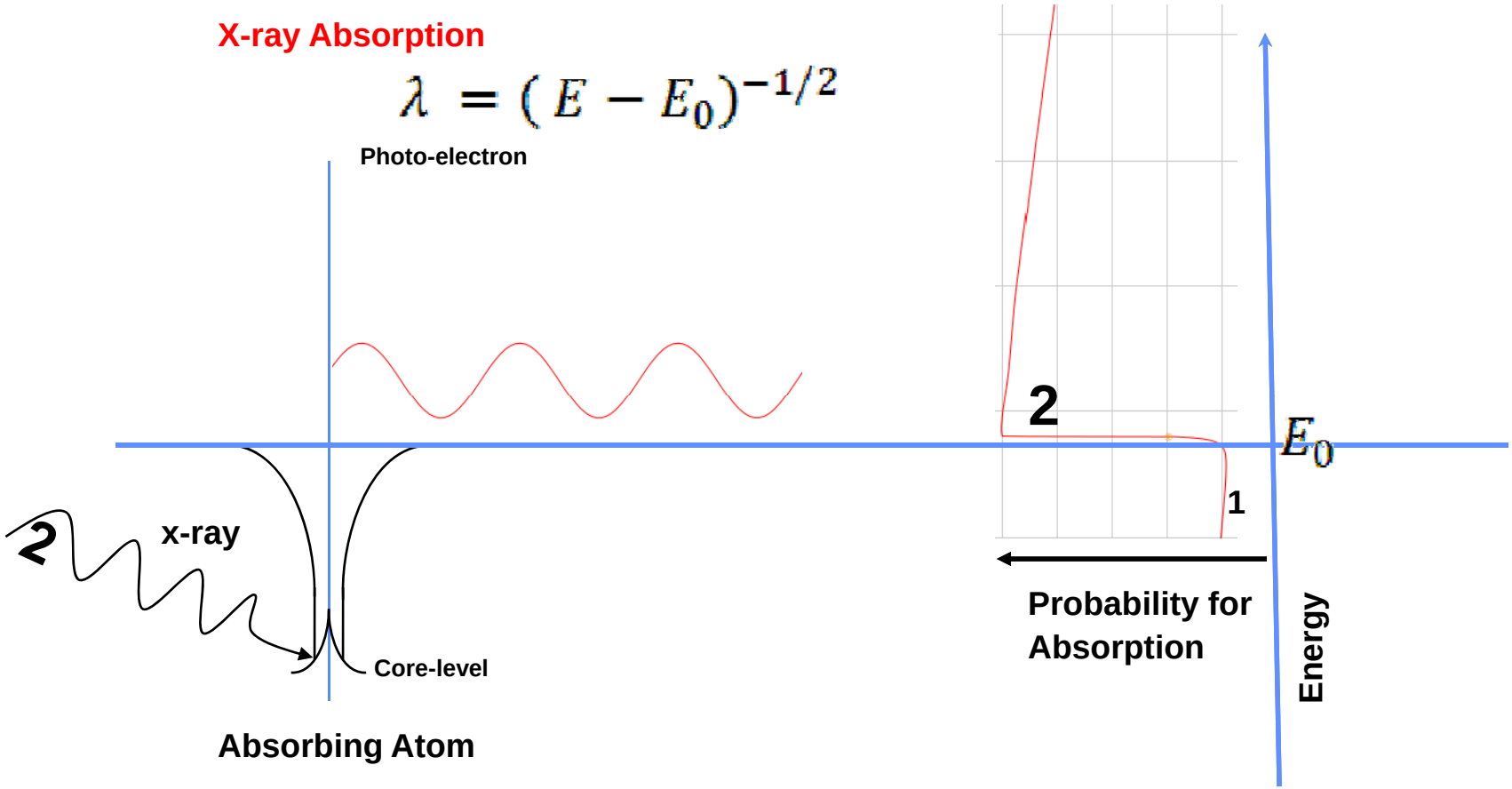
X-ray Absorption Process



- **#1: X-ray with energy below the binding energy of the core level does not interact with the atom**

***Presented by Matt Newville**

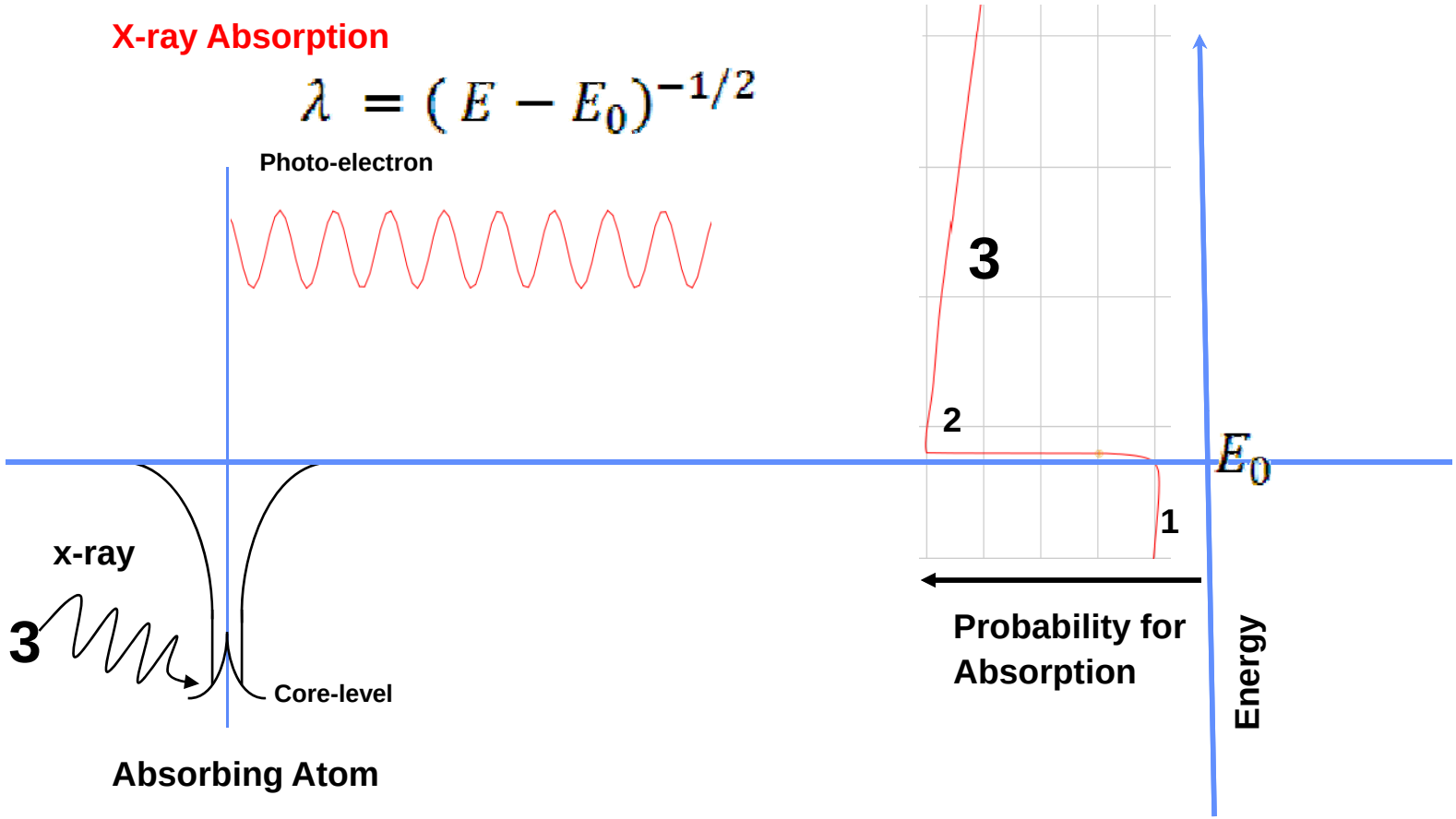
X-ray Absorption Process



- **#2: X-ray with energy just above the binding energy of the core level has a probability of being adsorbed producing a low energy photo-electron**

***Presented by Matt Newville**

X-ray Absorption Process



- #3) X-ray with higher energy have a probability of being adsorbed and producing higher energy photo-electron

*Presented by Matt Newville

Fermi's Golden Rule

$$\mu(E) \propto |\langle i|\mathcal{H}|f\rangle|^2$$

- **Transition between two quantum states**
- **Initial state is well localized at the absorbing atom**
- **Final state is not, but can be written in terms of two parts**

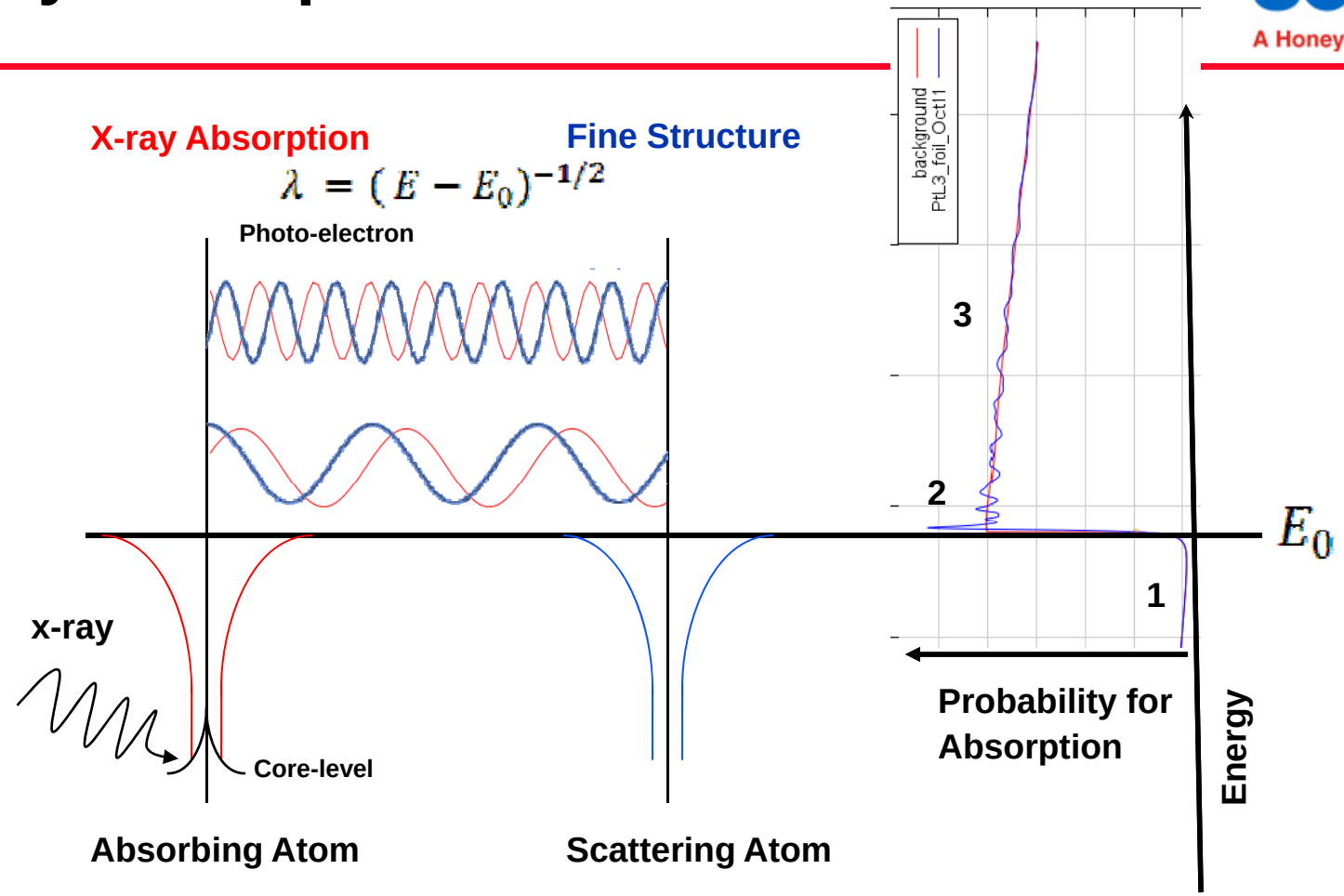
$$|f\rangle = |f_0\rangle + |\Delta f\rangle_{\text{neighboring atoms}}$$

$$\mu(E) = \mu_0(E)[1 + \chi(E)]$$

- **Probability for adsorption is the probability for an isolated atom multiplied by a perturbation due to neighboring atoms**

$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu(E)}$$

X-ray Absorption Fine Structure



- **Interference between outgoing and scattered photoelectron at the absorbing atom causes modulations in the probability for absorption.**

EXAFS Equation and Signal

Number of Neighbors

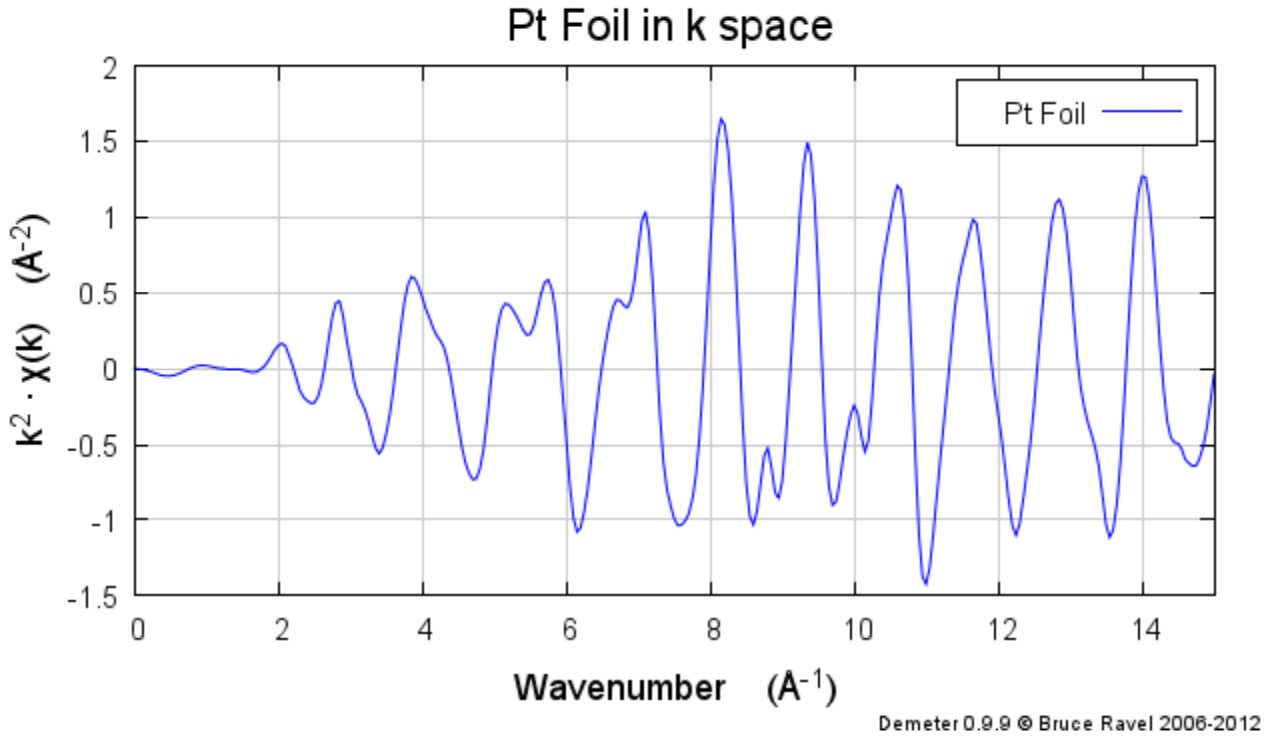
Scattering Amplitude

Disorder in interatomic distance

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2k^2\sigma_j^2}}{k\, R_j^2} \sin[2kR_j + \delta_j(k)]$$

Neighbor Distance

Atomic Phase Shift



- **EXAFS signal can be expressed as a sum of sine waves**

X-ray Absorption Near Edge Structure

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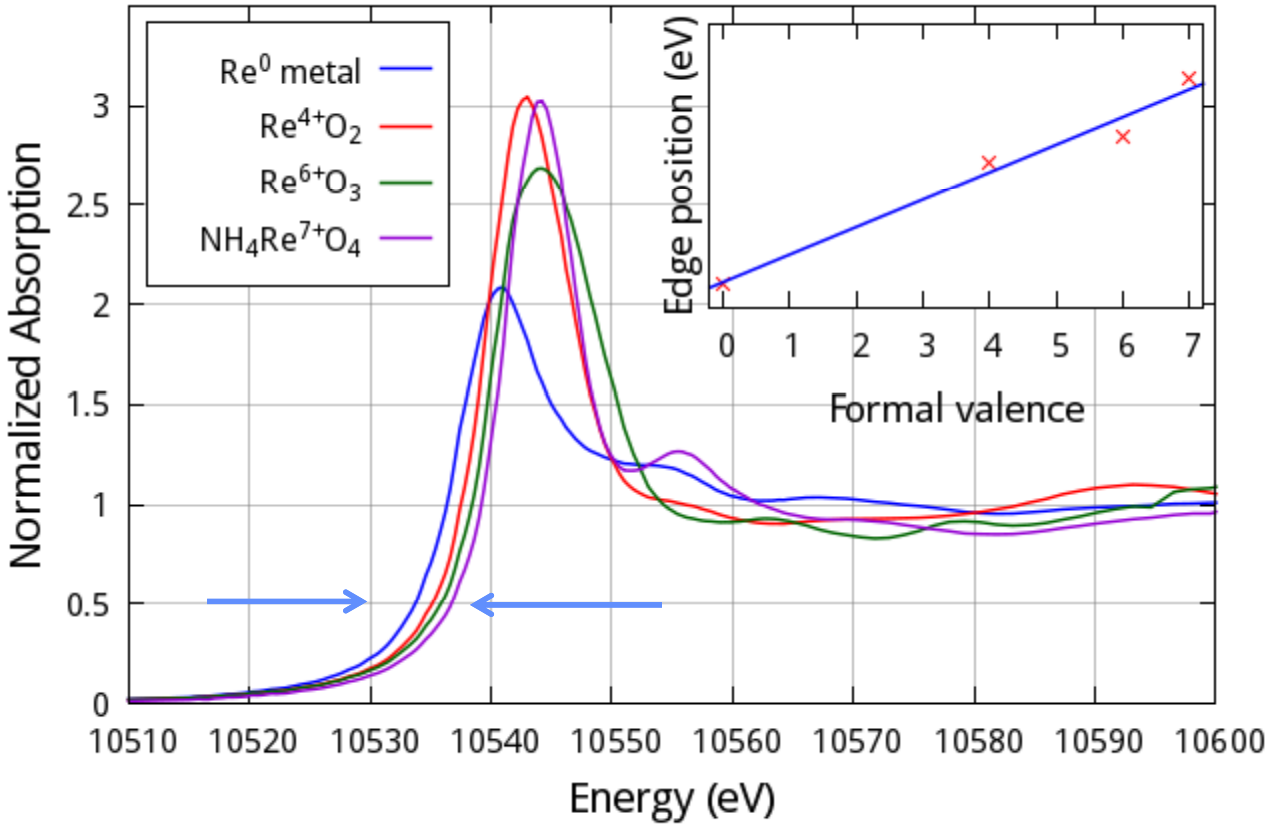
- **Analysis of XANES spectra**
  - **Assigning absorption edge energies to oxidation states**
  - **Linear combination fitting (LCF) using standard to reproduce the measured spectrum to determine the relative amount of each standard in the measured spectrum**
  - **Theoretical Calculations (FEFF8) using atomic clusters to calculate the absorption edge spectrum to reproduce key features and assign those features to specific atomic configurations**

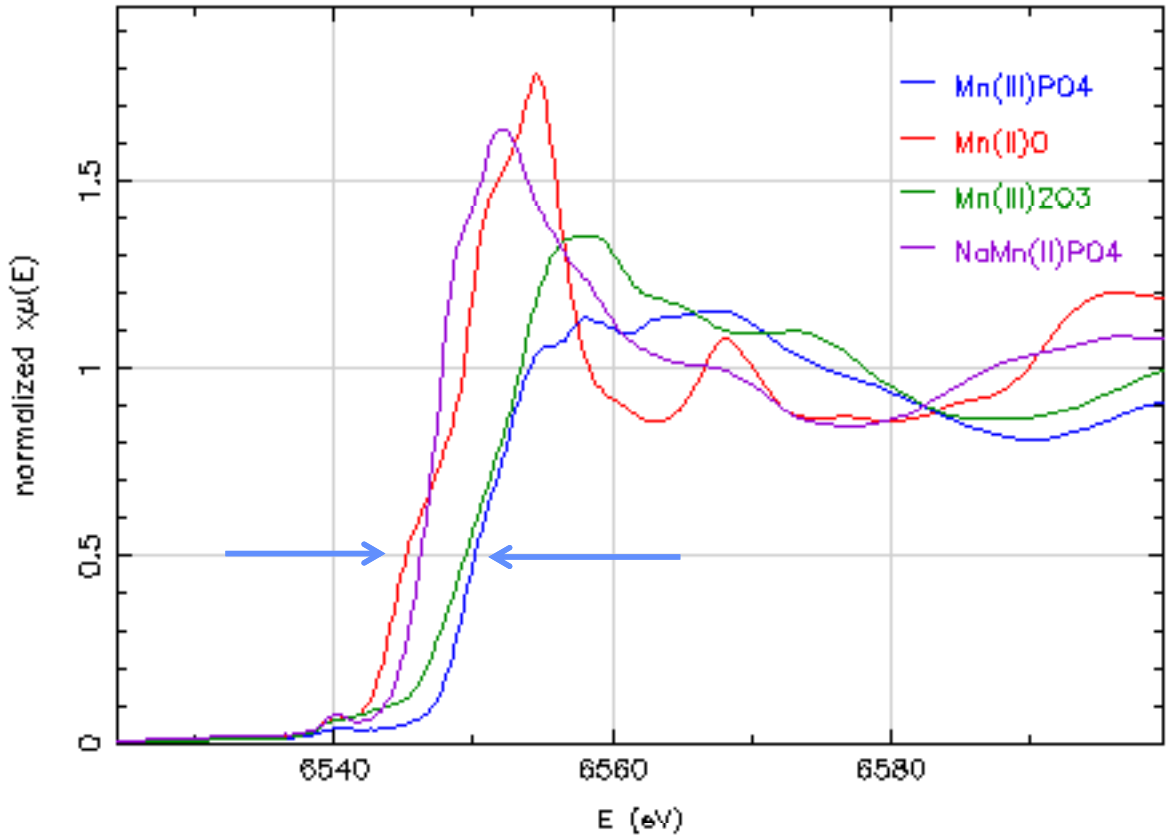
Edge Position and Valence State



- **For some materials the edge position can be calibrated to determine the average valence state**
- **As an element becomes more positively charged the x-ray energy needed to remove an additional electron is increased causing the edge to shift.**

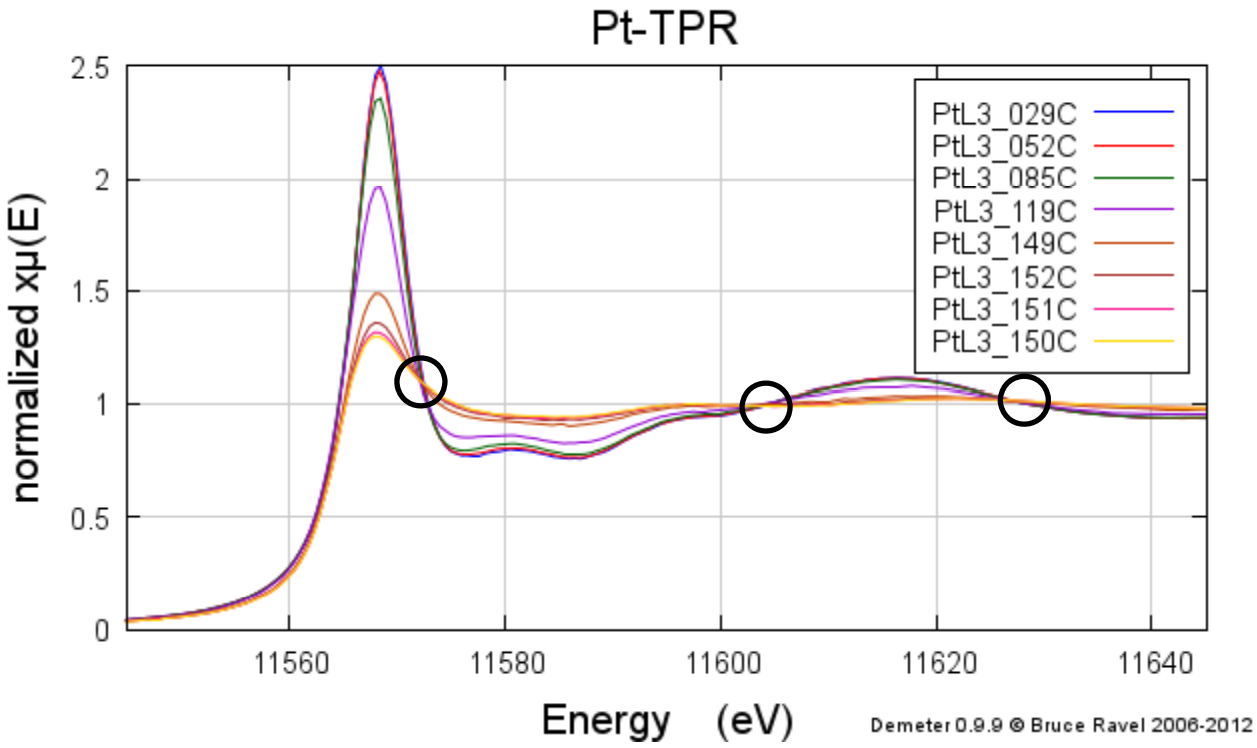
Journal syn rad 2010

Mn oxides and phosphates



- **Example were the edge position does not track cleanly with oxidation state**

Pt Data Series

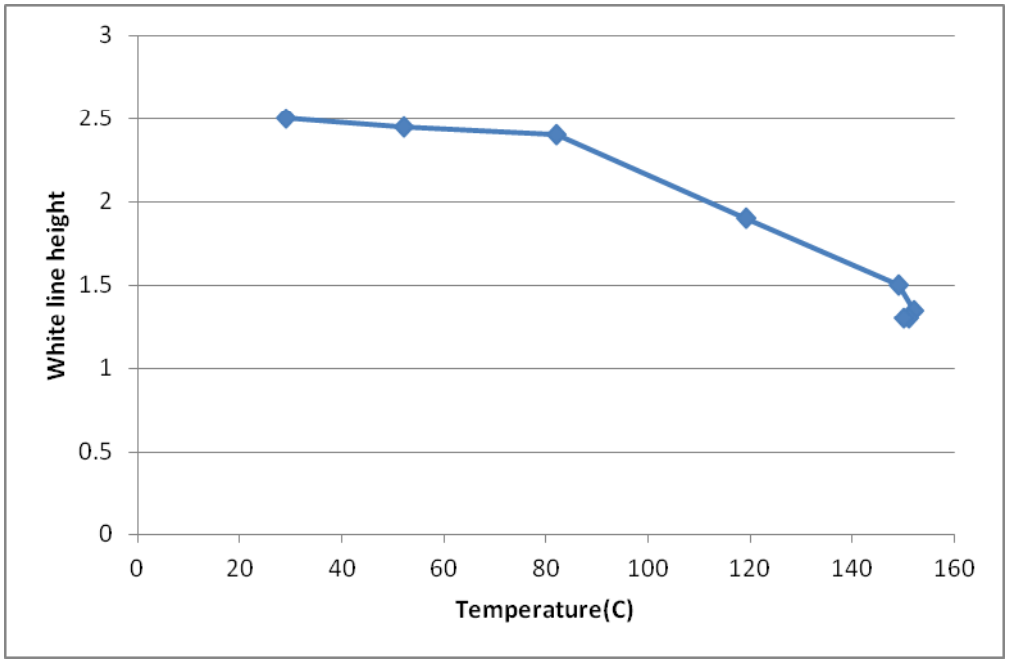


- **Data Series were Pt is being reduced in situ.**
- **Look for Isosbestic points in normalized XANES spectra**

Interpretation of XANES

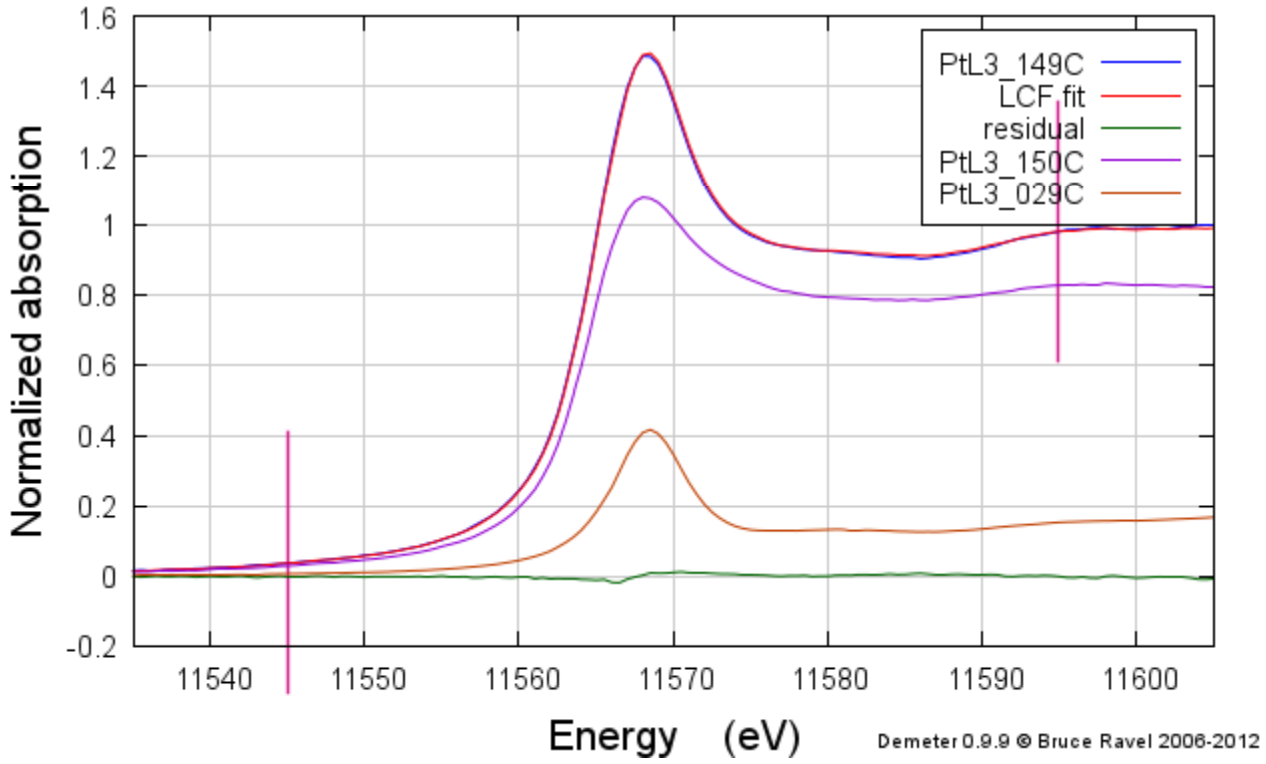
100% Oxidized?

100% Reduced?



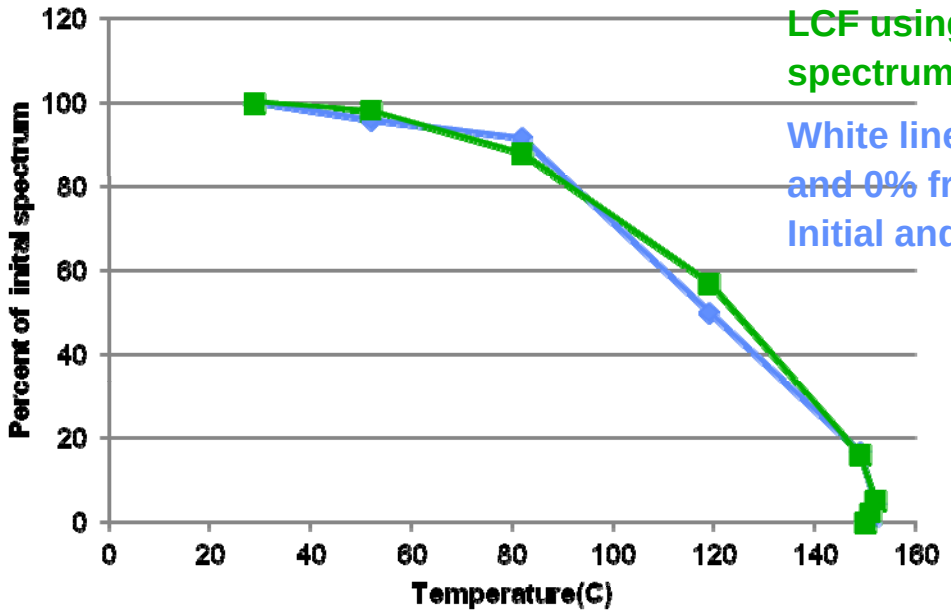
- Plot white line height with temperature to determine the rate of Pt reduction
- White line height: White line height is a measured of the unoccupied d-electrons

Linear Combination Fitting #1



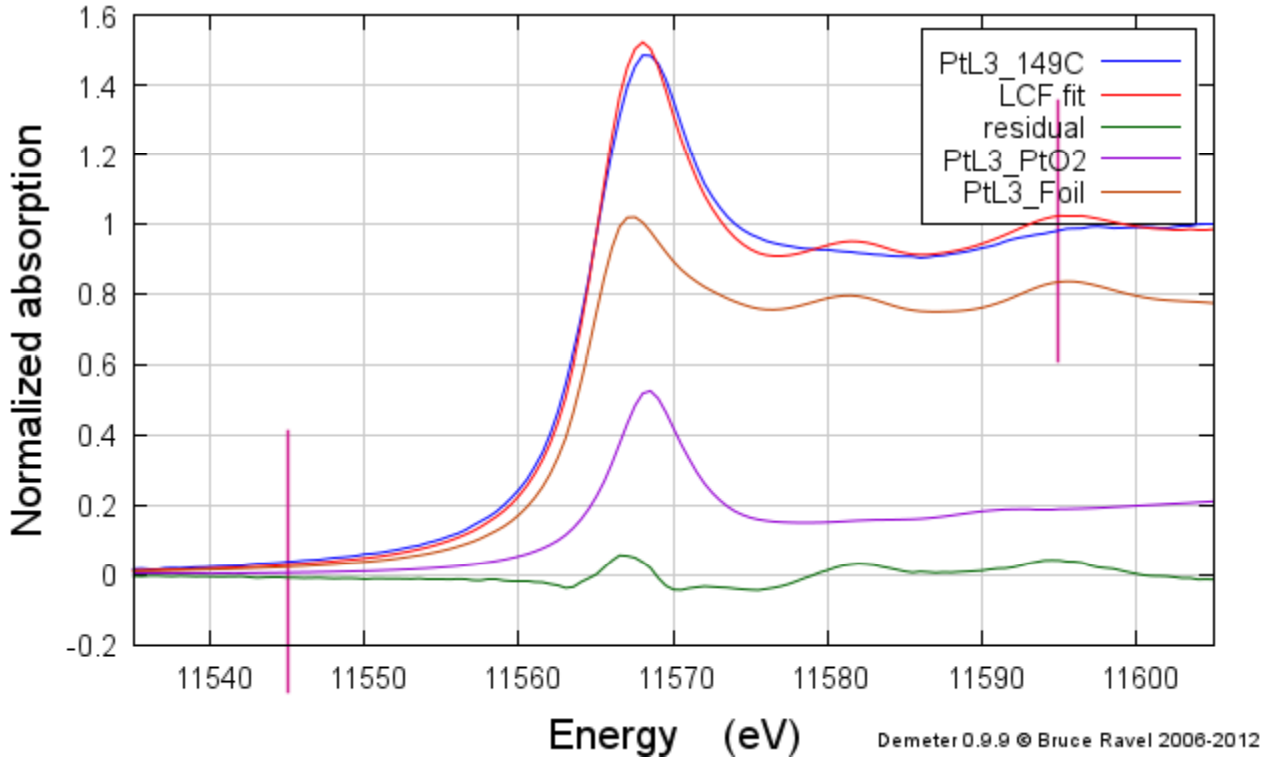
- **Fit 149ºC data with combination of 29ºC data and 150ºC data.**

Comparison of LCF and white line height



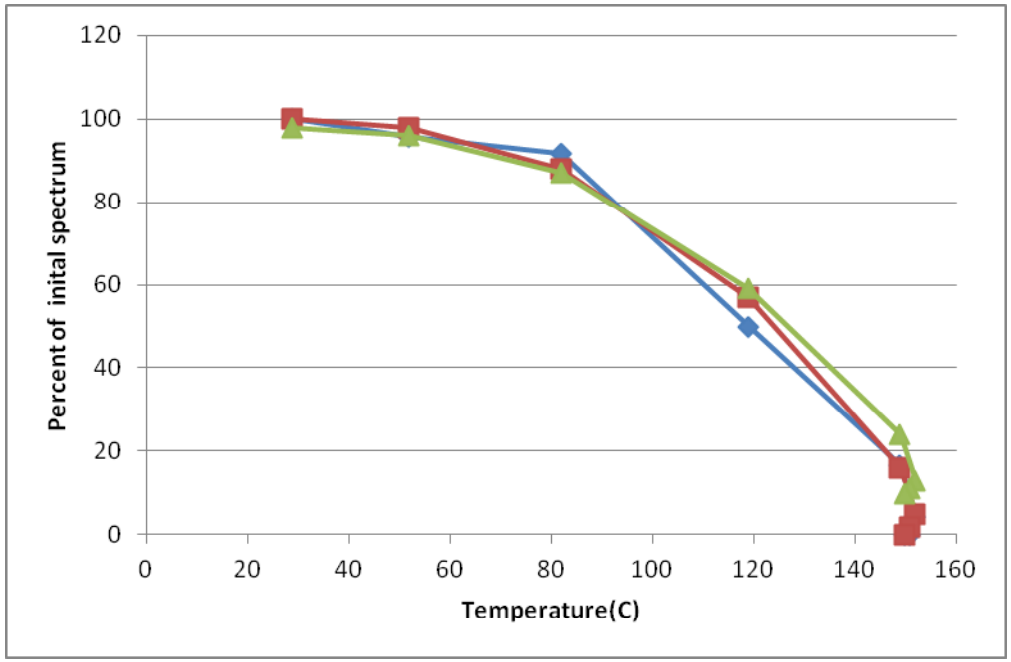
- Similar results for both methods of interpretation
- LCF: Assume speciation of Pt evolves from the initial species to the final species. No intermediate species present.
- White line height: Assume white line height the available d-electrons .

Linear Combination Fitting #2



- **Linear combination fitting using PtO_2 and Pt foil as a standards**

Comparison of Fitting Results



White line height scaled to 100% and 0% from Initial and final spectrum

LCF using initial and final spectrum

LCF using PtO2 and Ptfoil

- All three methods give similar results.
- Largest source of error comes from incomplete knowledge of chemical speciation before, during and after in situ measurement.
- LCF using standards assumes that these standards are a good representation of Pt speciation in sample.

Modeling EXAFS Spectra

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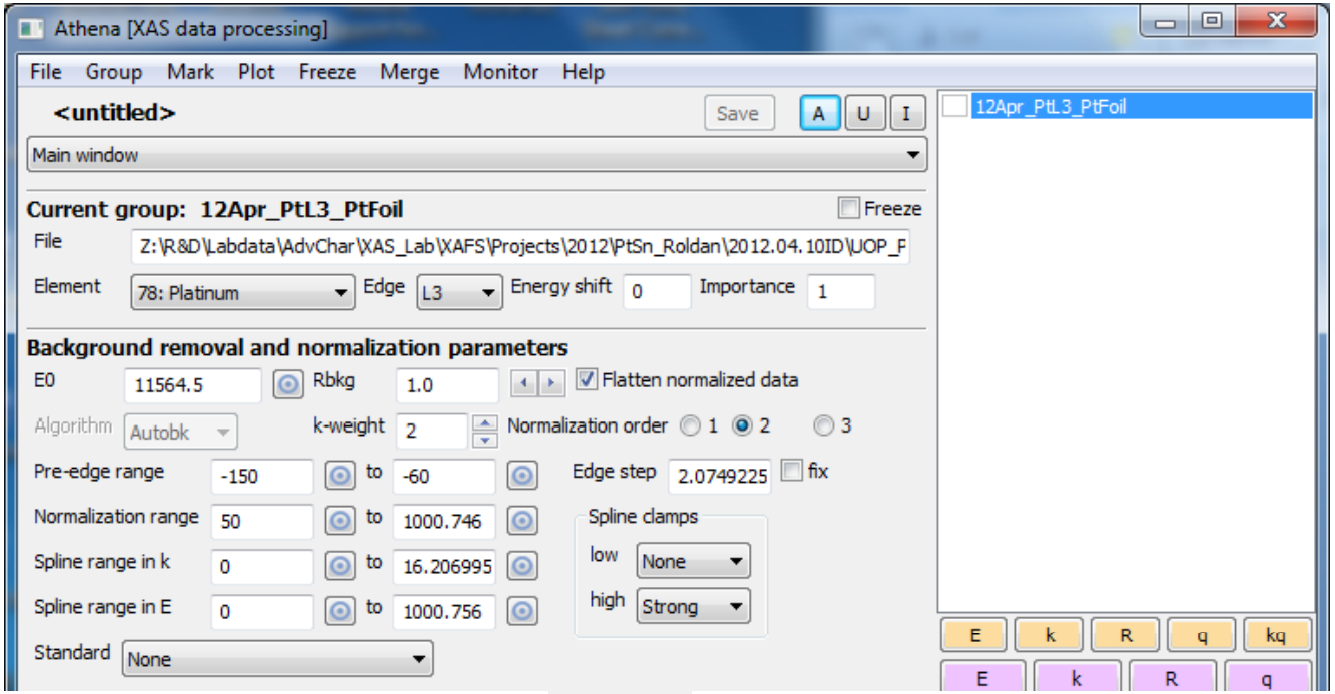
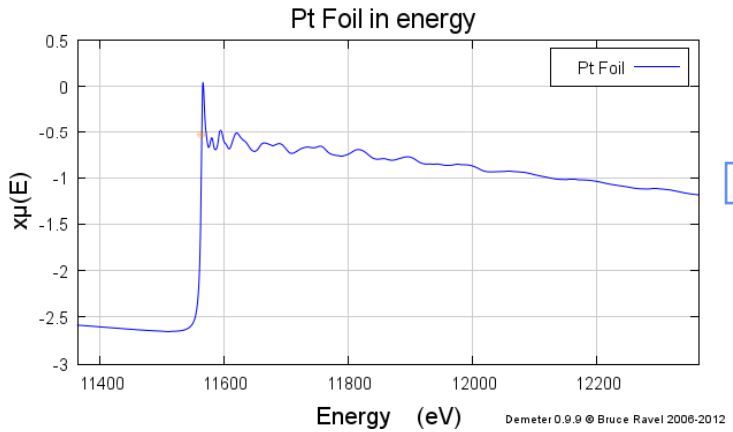
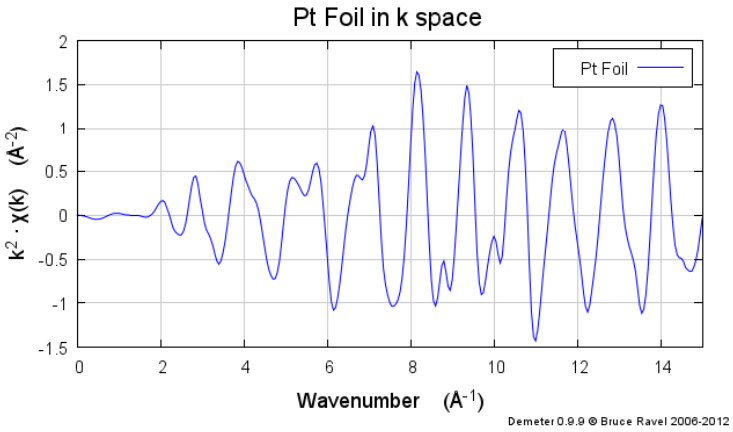
- **Introduction to Athena (Background removal)**
- **Introduction to Artemis (EXAFS Modeling)**
  - **Modeling Cu foil**
  - **Modeling U to determine neighboring atom type**
  - **Multiple data set modeling**

- 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.

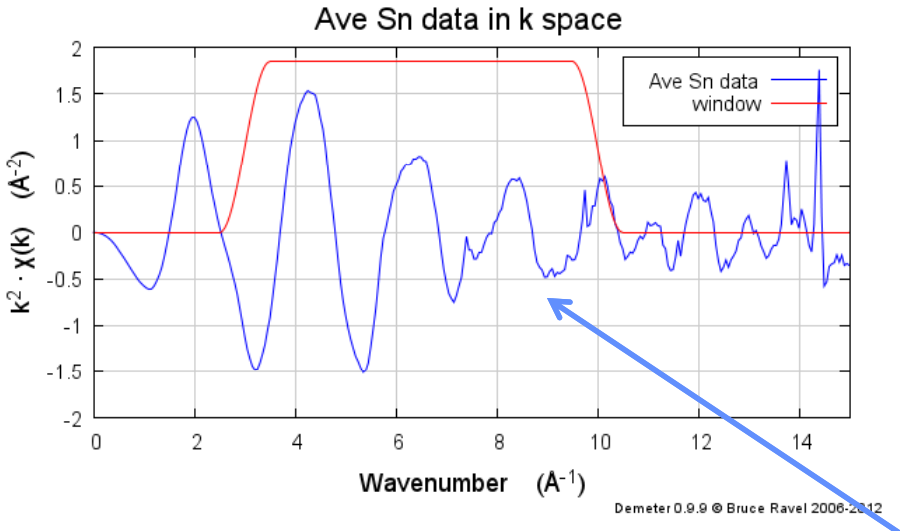
Athena: Background Removal

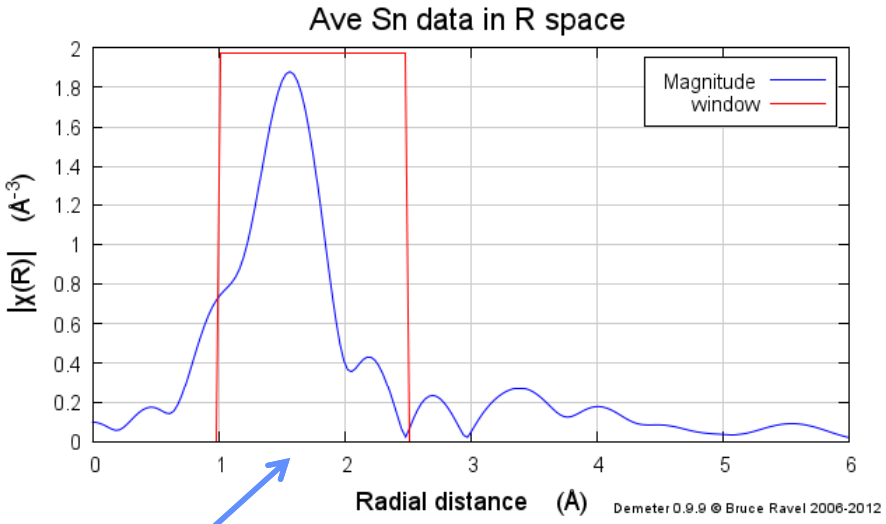






Information Content in Data Set





Nyquist cirterion: $N_{idp} \approx \frac{2\,\Delta k \Delta R}{\pi}$

- **Number of independent points is proportional to the data range used in FT and the fitting range.**
- **Cannot have more variables determined in a fit than the number of independent points**

Comparison of Models

χ^2 : sum of the difference between the data and the theory

$$\chi^2 = \frac{N_{idp}}{\epsilon N_{data}} \sum_{i=min}^{max} [Re(\chi_d(r_i) - \chi_t(r_i))^2] + Im(\chi_d(r_i) - \chi_t(r_i))^2]$$

$$\epsilon = measurement\ uncertainty$$

$$\chi_\nu^2 = \frac{\chi^2}{\nu}$$

Reduced χ^2 : sum of the difference between the data and the theory, scaled by the number of independent points. $\nu = N_{idp} - N_{var}$
Useful for comparing models with different number of variables

R-factor: fractional misfit

$$\mathcal{R} = \frac{\sum_{i=min}^{max} [\, Re(\chi_d(r_i) - \chi_t(r_i))^2 + Im(\chi_d(r_i) - \chi_t(r_i))^2 \,]}{\sum_{i=min}^{max} [\, Re(\chi_d(r_i))^2 + Im(\chi_d(r_i))^2 \,]}$$

- FEFFIT uses Levenberg-Marquardt non-linear least-squares minimization
- χ_ν^2 are used to compare between two different models. χ_ν^2 values are poorly scaled and often 100 – 1000. χ_ν^2 need to change by more than a factor of 2 to be significant.
- Error bars are scaled by $\sqrt{\chi_\nu^2}$, assuming that the model is good.

Building Theoretical Model: Atoms page

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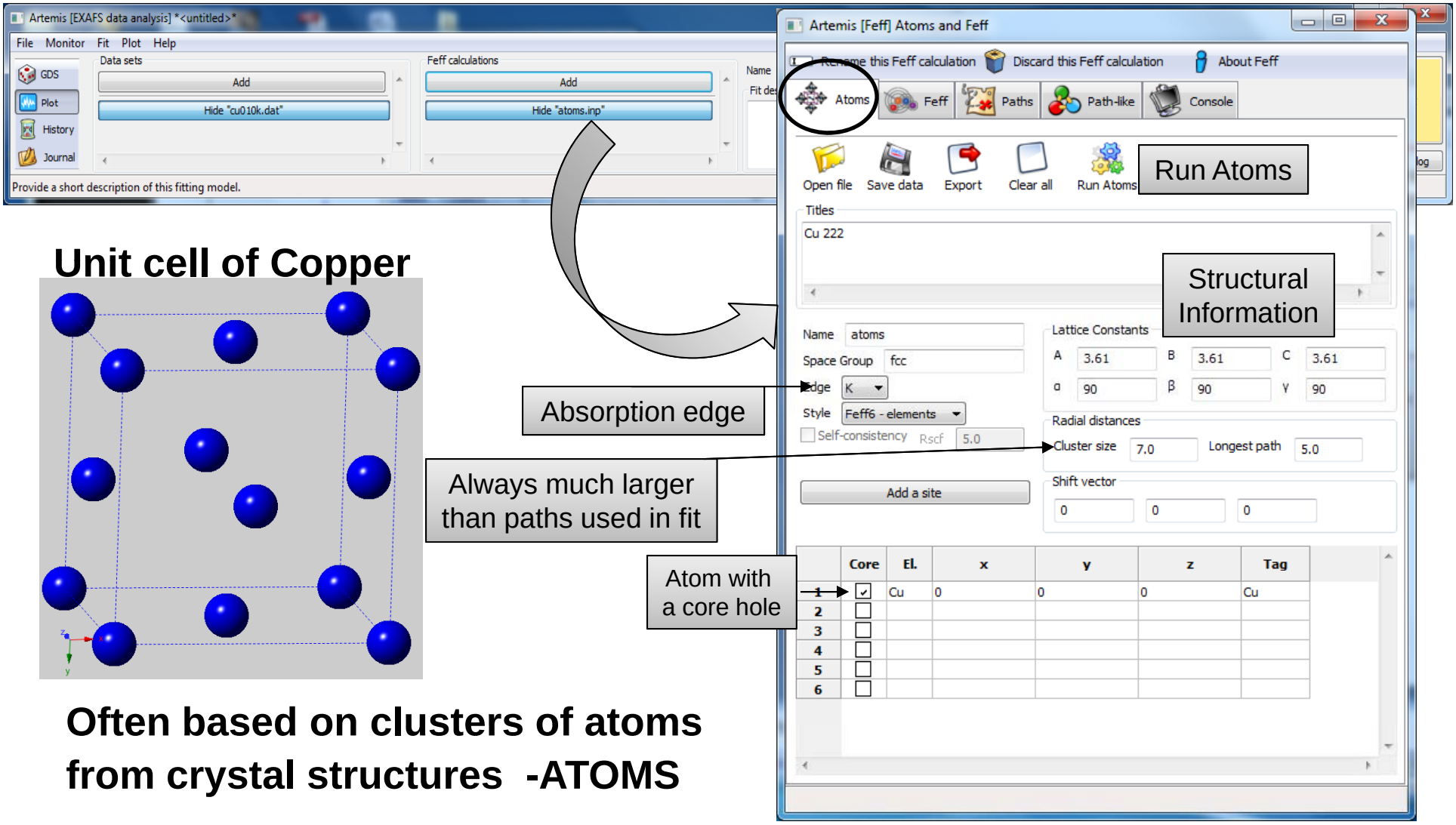
➢File: open file: F:\Ifeffit\examples\Artemis\Cu\atoms.inp

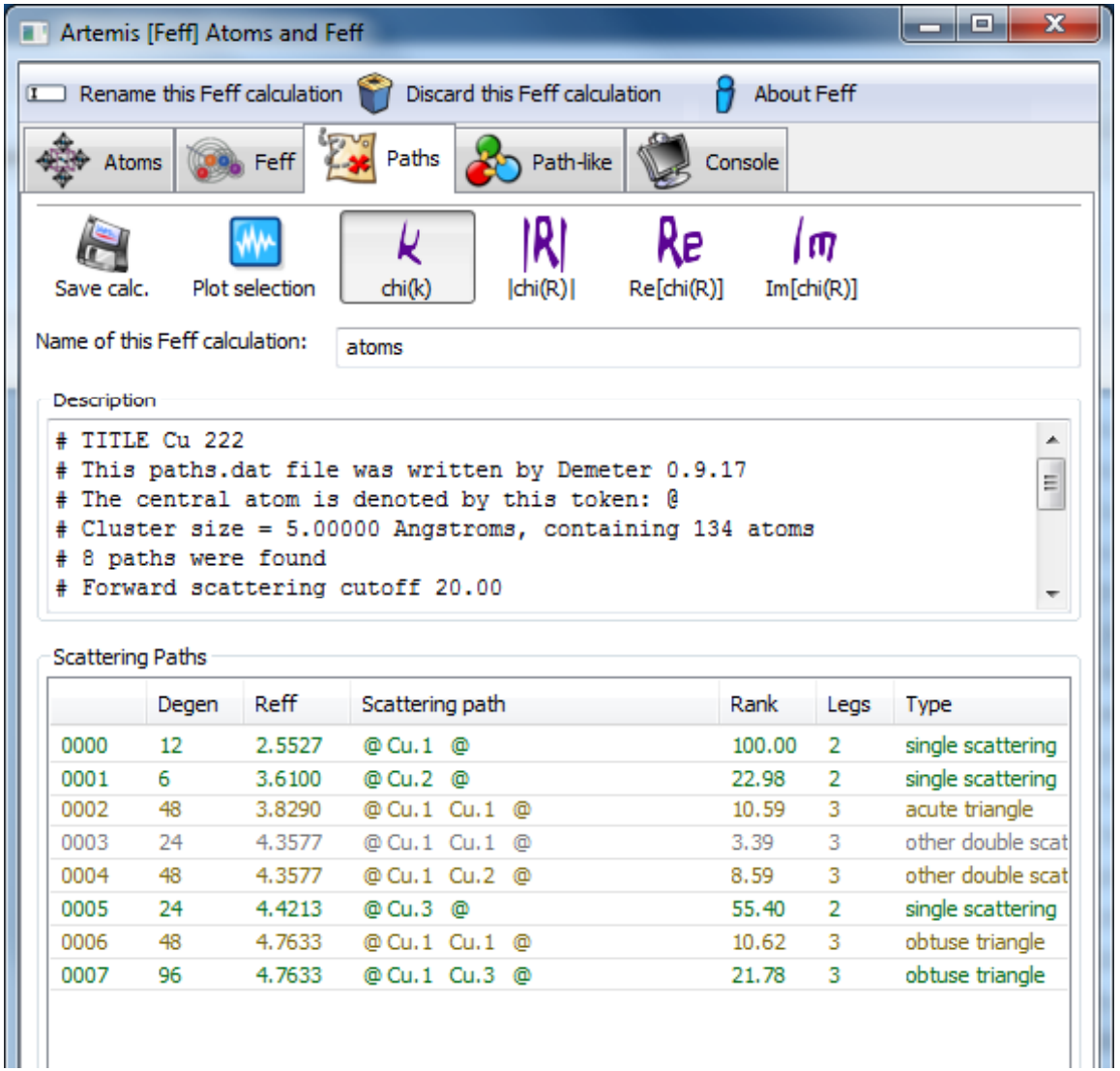


Unit cell of Copper

Often based on clusters of atoms from crystal structures -ATOMS

Feff Scattering Paths

- **Degen:** **Degeneracy of the path (number of identical scattering paths)**
- **Reff:** **Inital half path length (bond length for single scattering path)**
- **Rank:** **Estimate of amplitude of path relative to first path.**
- **Type:** **Description of the scattering path.**
- **scattering path:** **atoms scattering photoelectron, [@] symbol represents core atom.**



	Degen	Reff	Scattering path	Rank	Legs	Type
0000	12	2.5527	@ Cu.1 @	100.00	2	single scattering
0001	6	3.6100	@ Cu.2 @	22.98	2	single scattering
0002	48	3.8290	@ Cu.1 Cu.1 @	10.59	3	acute triangle
0003	24	4.3577	@ Cu.1 Cu.1 @	3.39	3	other double scat
0004	48	4.3577	@ Cu.1 Cu.2 @	8.59	3	other double scat
0005	24	4.4213	@ Cu.3 @	55.40	2	single scattering
0006	48	4.7633	@ Cu.1 Cu.1 @	10.62	3	obtuse triangle
0007	96	4.7633	@ Cu.1 Cu.3 @	21.78	3	obtuse triangle

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.

The EXAFS Equation

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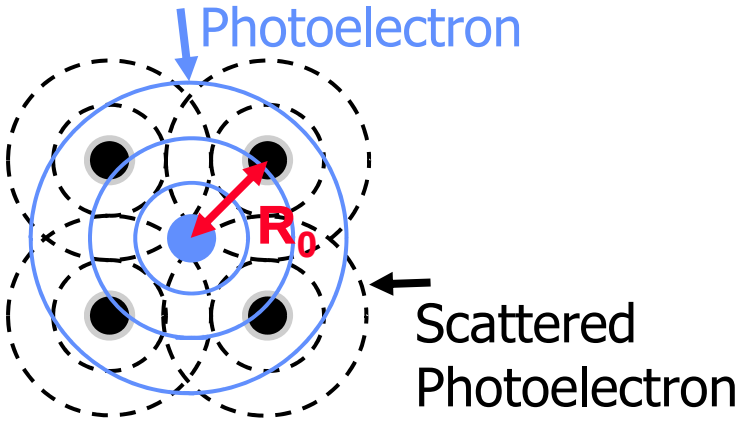
- E. A. Stern and S M Heald Basic principles and applications of EXAFS. Handbook of Synchrotron Radiaction. E. E. Koch. New York, North-Holland. **10:** pp 995-1014, 1983.
- E. A. Stern. "Theory of the extended x-ray-absorption fine structure." Phys Rev B **10**(8): pp 3027-3037, Oct 1974.
- E A Stern. "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:

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

$$R_i = R_0 + \Delta R$$

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

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

Parameters often determined from a fit

- 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.

Models to consider:

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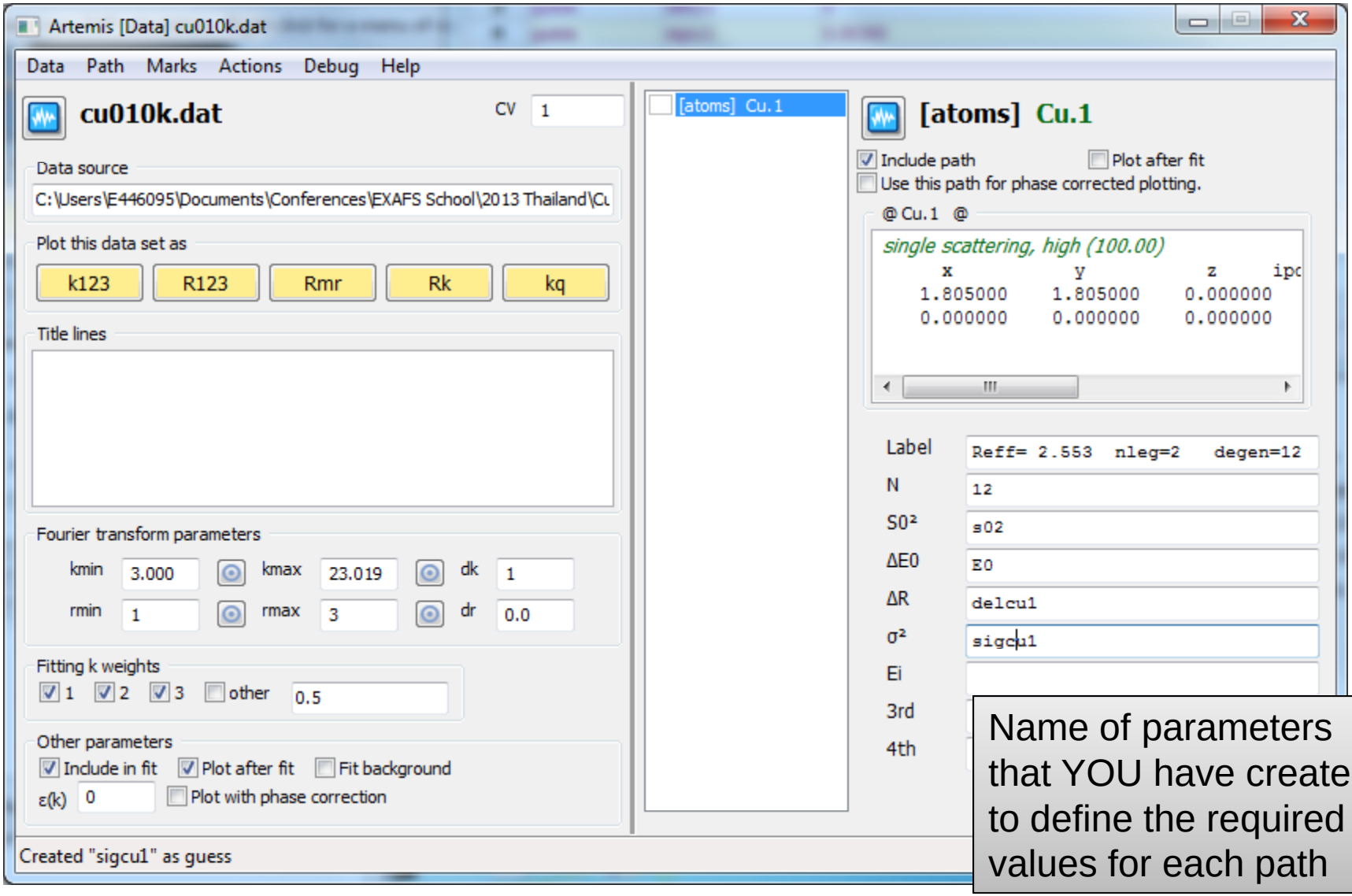
- Δr:
  - Symmetric expansion term: Alpha * reff.
  - Grouped depending on distance and atom types
  - Related to unit cell dimensions
- ΔE:
  - Energy shifts that depend on atom type
  - One energy shift for all paths
  - Two energy shifts, one for first shell and another for all other shells
- σ^2: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

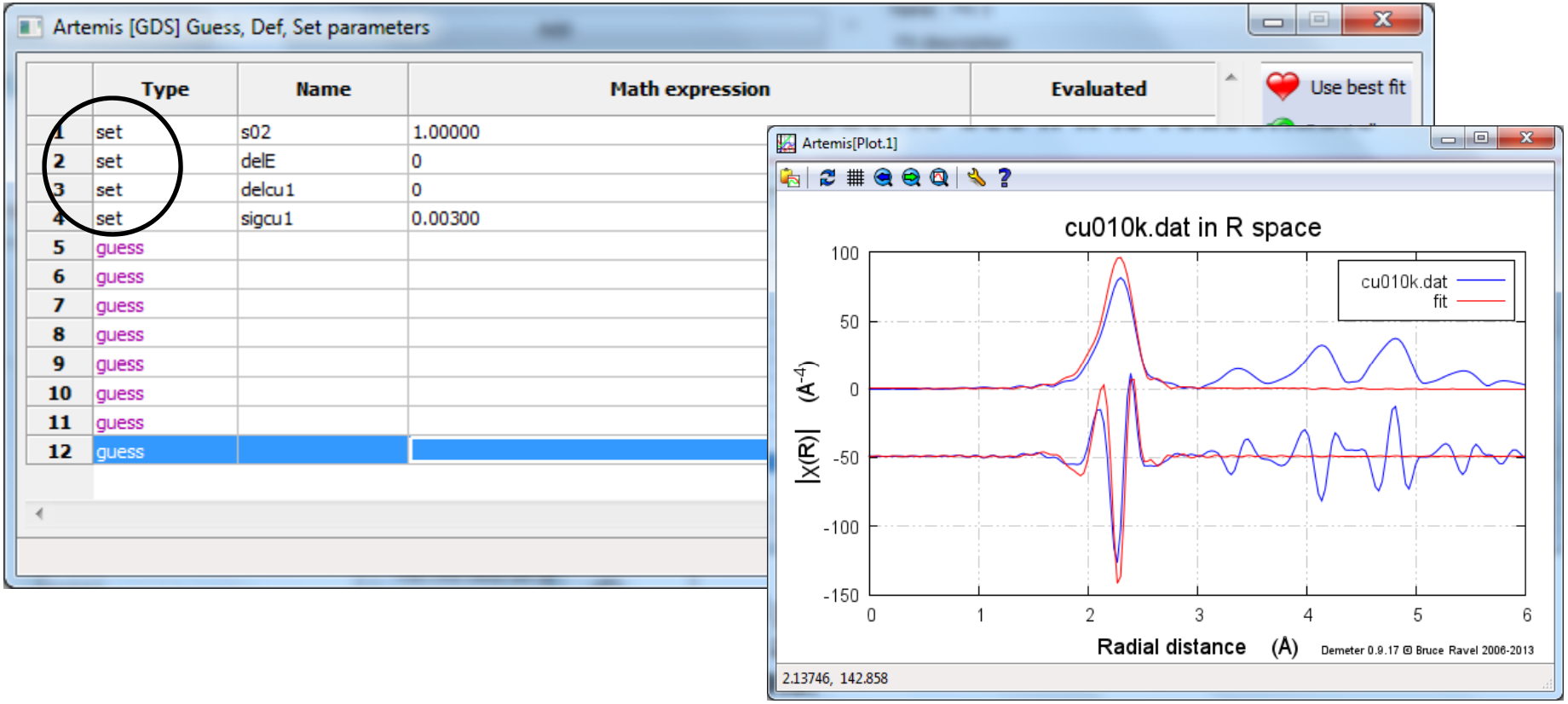
EXAFS parameters



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

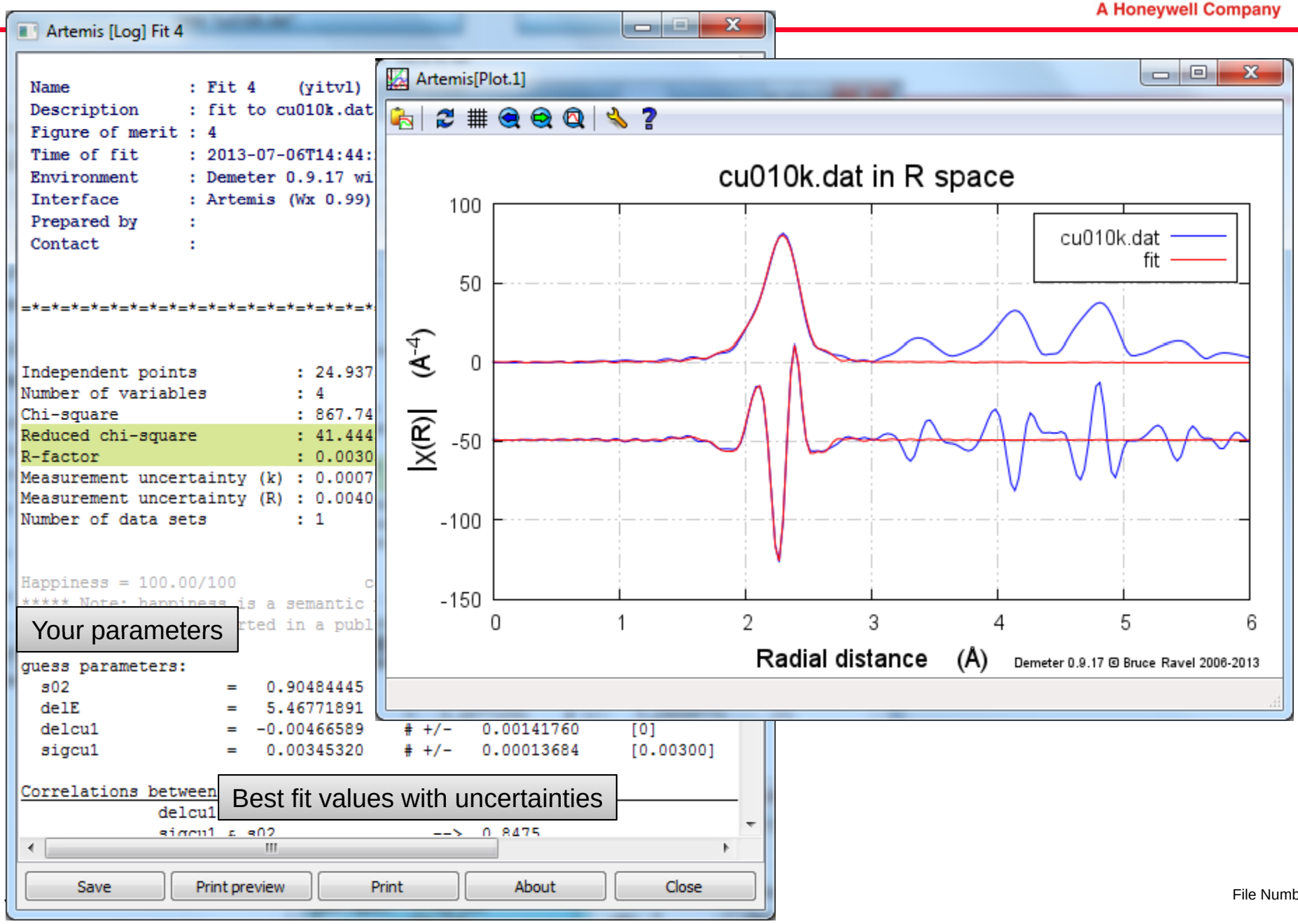
➢Click “Fit” to optimize these values

Check Model



- **Good practice: Set all parameters to a reasonable value and run a "fit" to see if the model is close to the data.**

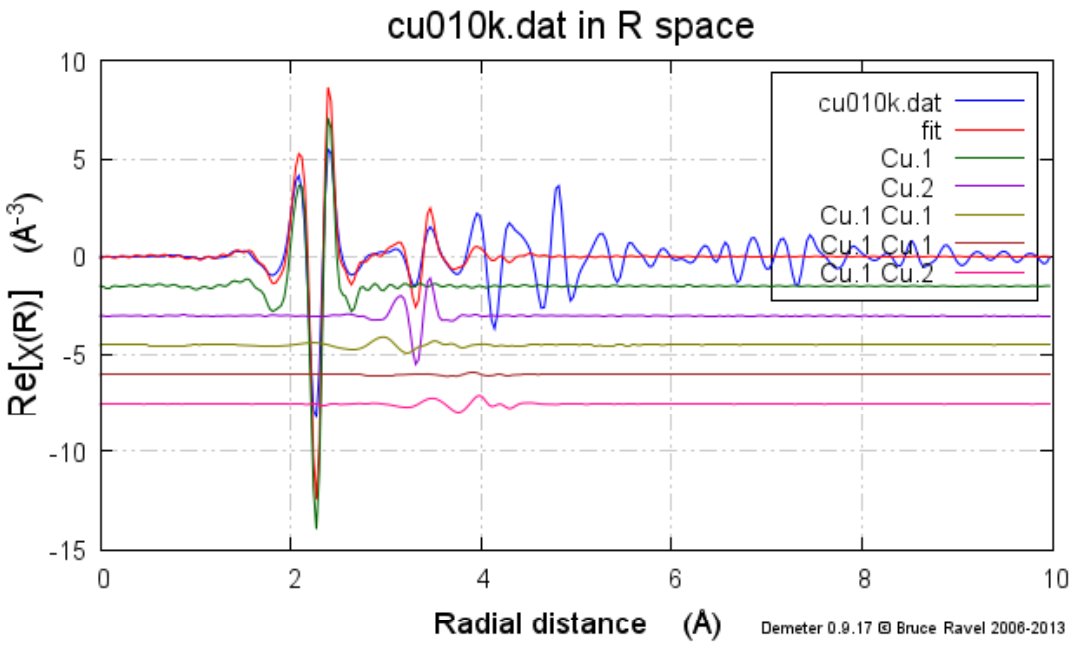
Fit Results



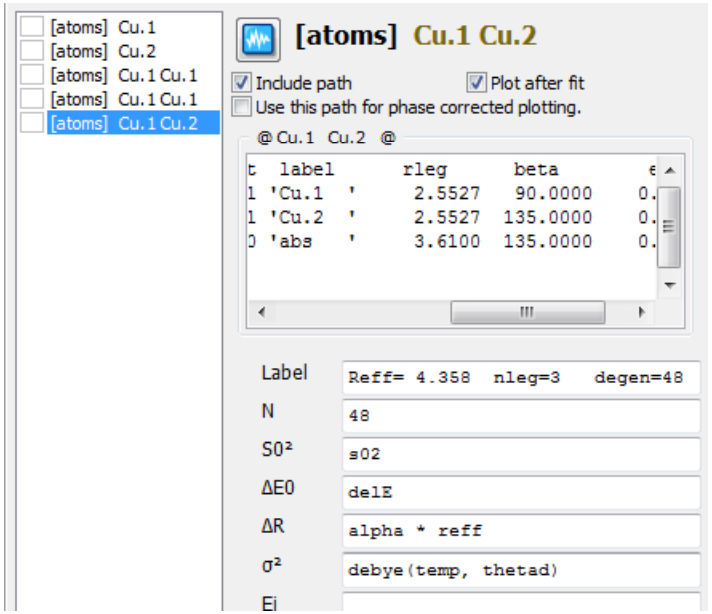
Your parameters

Best fit values with uncertainties

Cu: Three Shell Model



Path Info



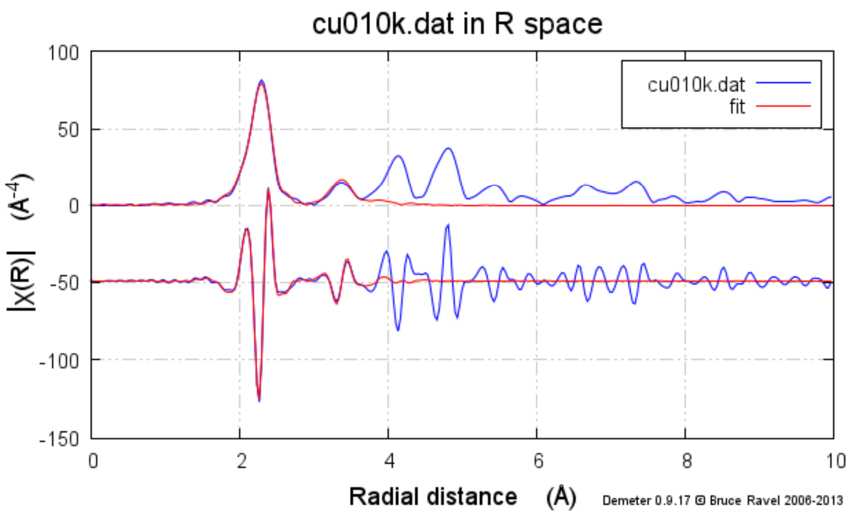
- Use alpha to define path lengths
- Use Debye temperature to define σ^2 values
- Each single scattering path fits into a specific signal in the data
- Check model by adding up all set parameters

GSD Info

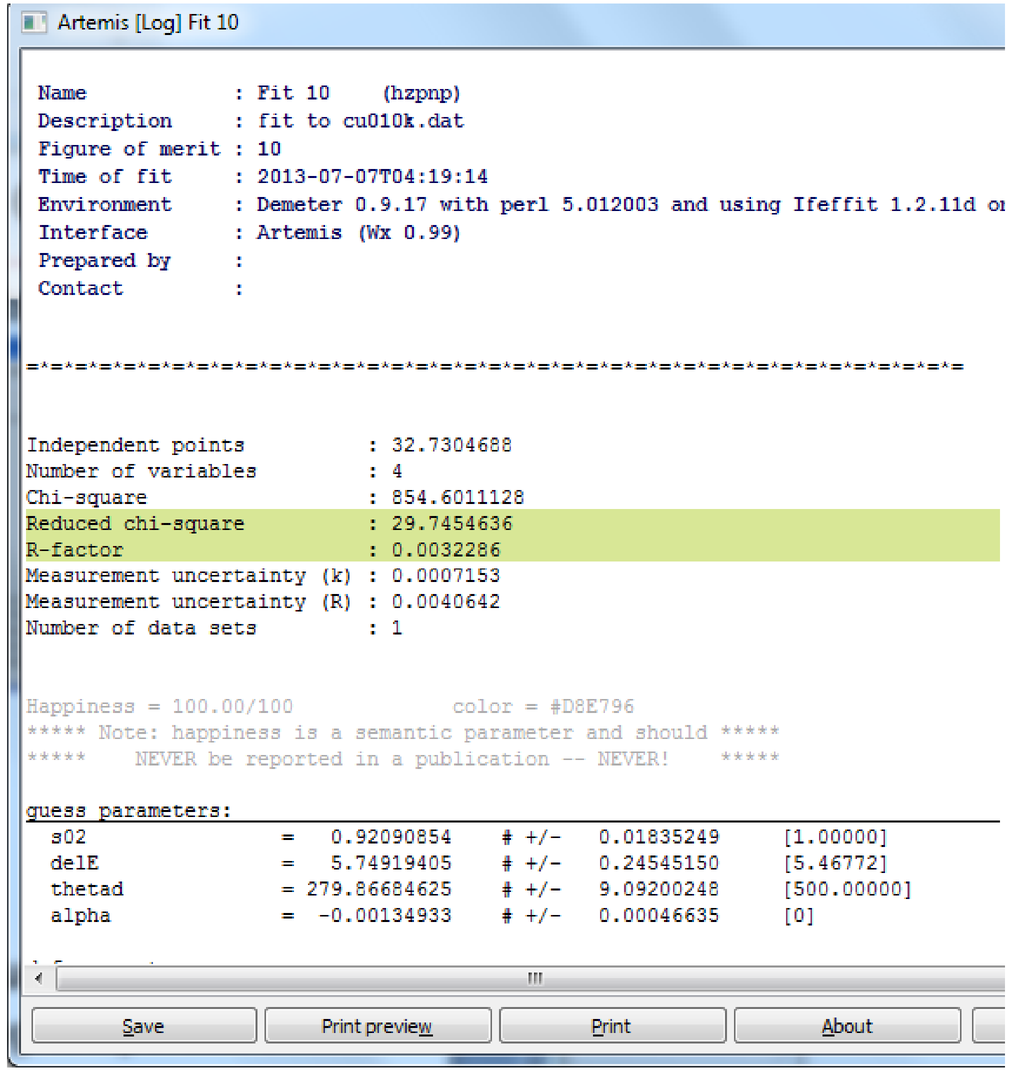
Artemis [GDS] Guess, Def, Set parameters

	Type	Name	Math expression
1	set	s02	1.00000
2	set	delE	5.46772
3	set	sigcu1	0.00300
4	set	temp	10
5	set	thetad	500.00000
6	set	alpha	0
7	guess		

Fitting results for three shell fit to Cu



Results Info


Artemis [Log] Fit 10

```
Name           : Fit 10     (hzpnp)
Description    : fit to cu010k.dat
Figure of merit : 10
Time of fit    : 2013-07-07T04:19:14
Environment    : Demeter 0.9.17 with perl 5.012003 and using Ifeffit 1.2.11d o
Interface      : Artemis (Wx 0.99)
Prepared by    :
Contact        :

=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=*=

Independent points          : 32.7304688
Number of variables         : 4
Chi-square                  : 854.6011128
Reduced chi-square          : 29.7454636
R-factor                    : 0.0032286
Measurement uncertainty (k) : 0.0007153
Measurement uncertainty (R) : 0.0040642
Number of data sets         : 1

Happiness = 100.00/100            color = #D8E796
***** Note: happiness is a semantic parameter and should *****
*****    NEVER be reported in a publication -- NEVER!    *****

guess parameters:
  s02             =    0.92090854   # +/-   0.01835249     [1.00000]
  delE            =    5.74919405   # +/-   0.24545150     [5.46772]
  thetad          =  279.86684625   # +/-   9.09200248     [500.00000]
  alpha           =   -0.00134933   # +/-   0.00046635     [0]
```

Save | Print preview | Print | About

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

Some EXAFS references

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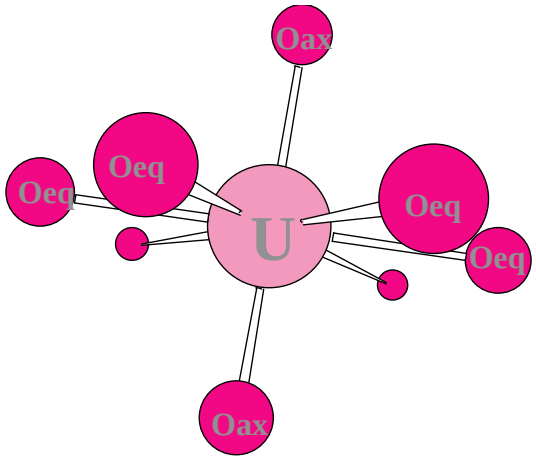
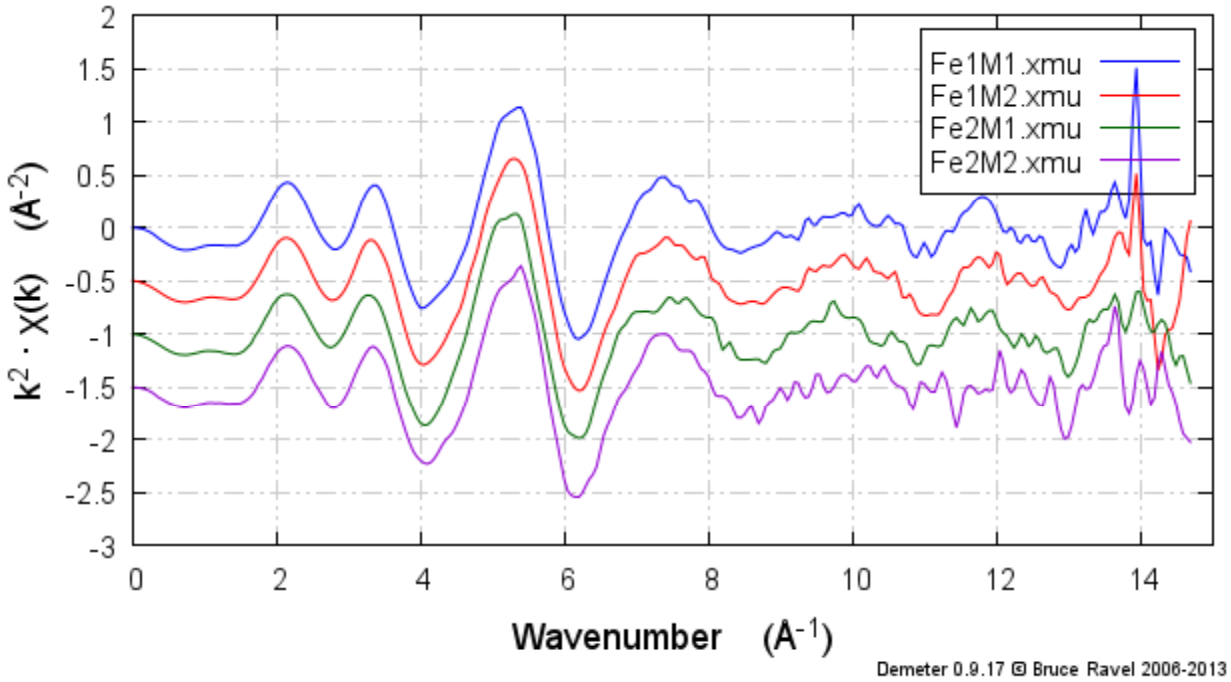
- Multiple edges, structural information: **B Ravel, E. Cockayne, M. Newville and K. M. Rabe. "Combined EXAFS and first-principles theory study of Pb1-xGexTe." Phys. Rev. B** 60**(21): pp 14632–14642, Dec 1999**
- Structural information, bond angles: **A. I. Frenkel, E A Stern, A. Voronel, M. Qian and 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.**
- **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.**

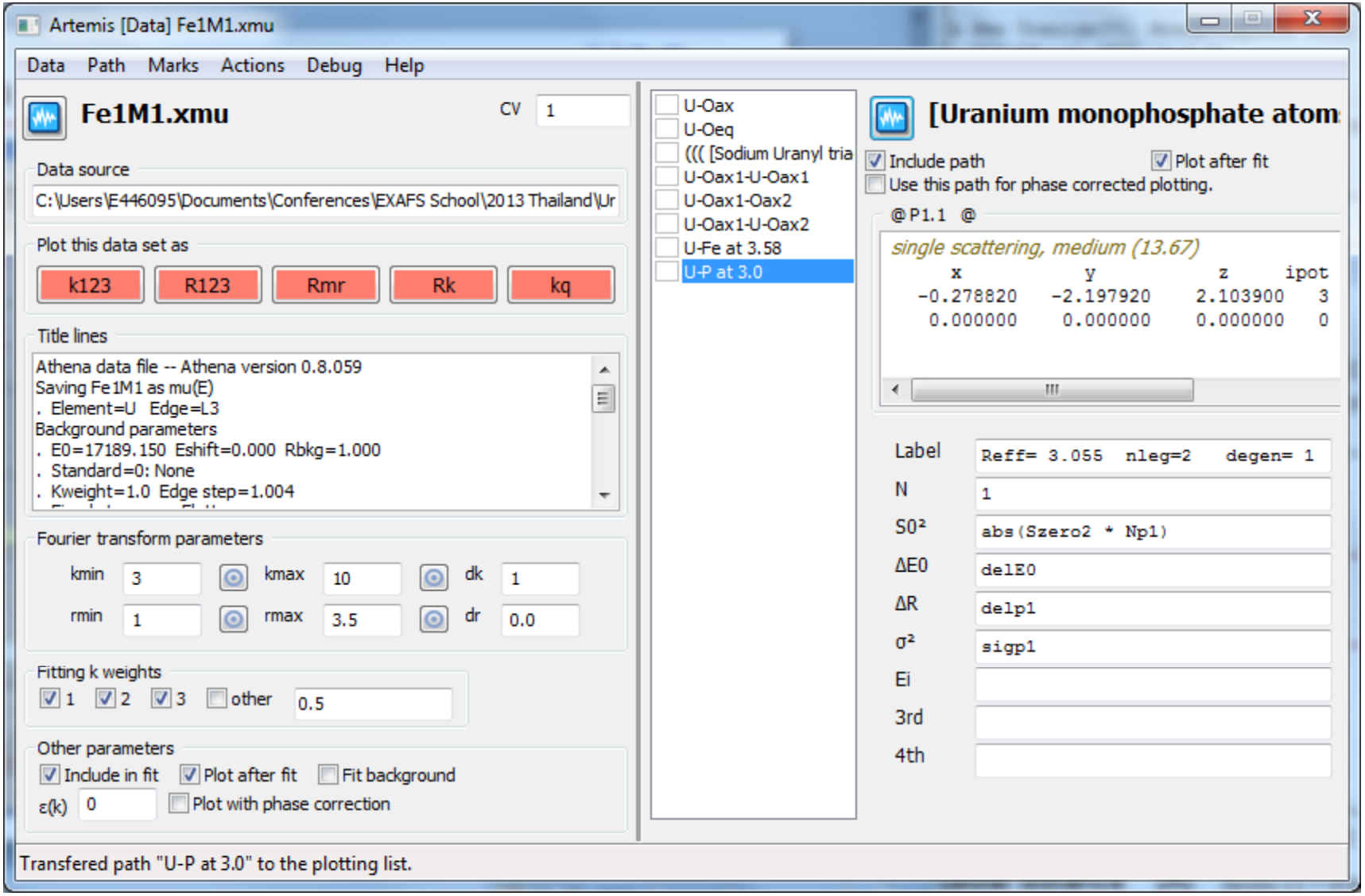
Determining 2nd shell atom type and number

- 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

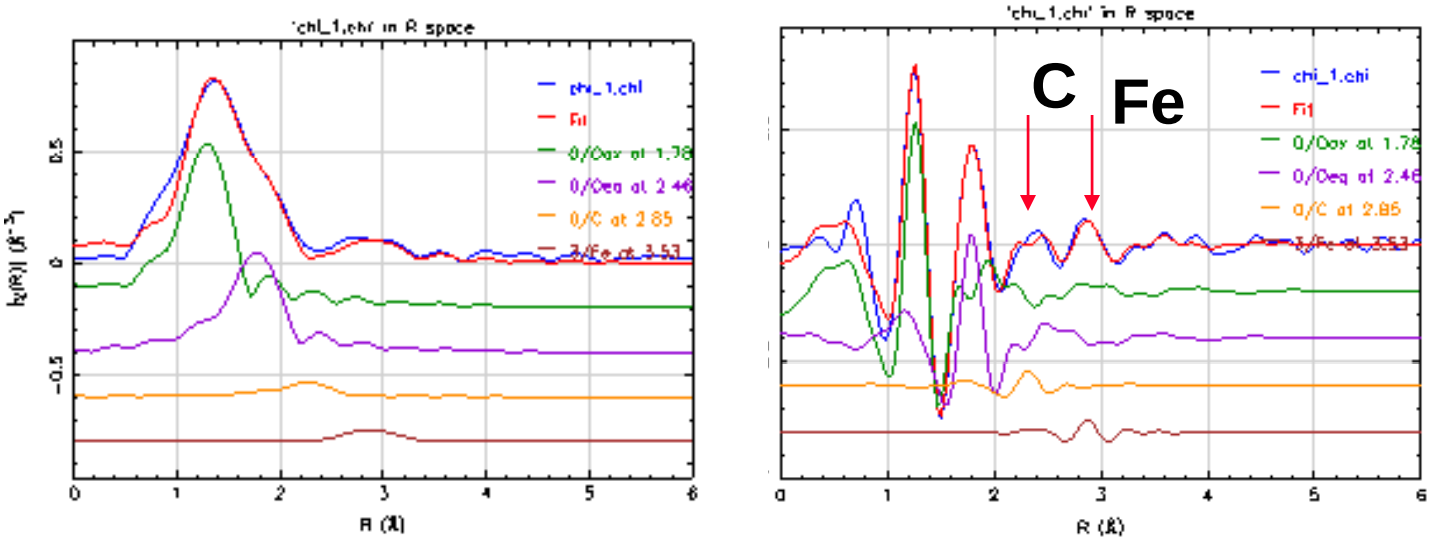




Setting up a Uranyl Model

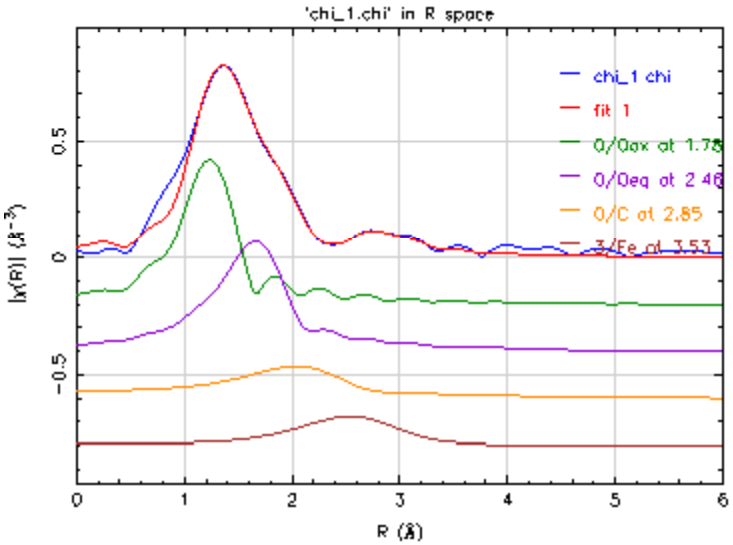


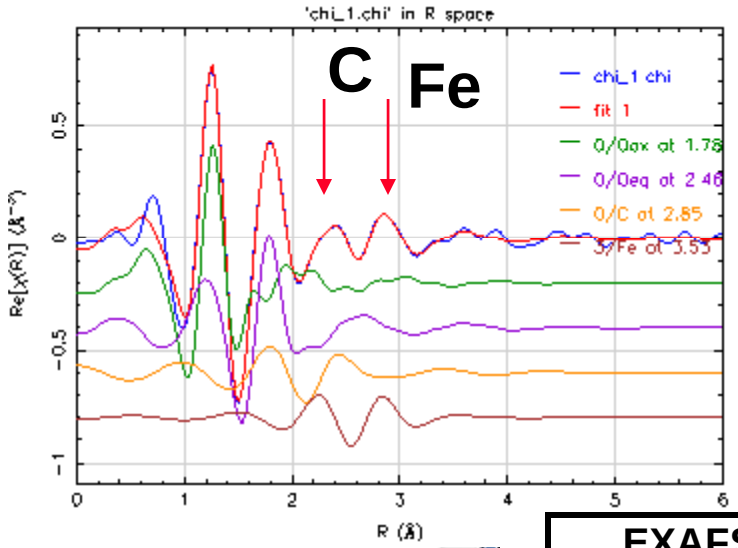
Test data for C and Fe shells



- **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



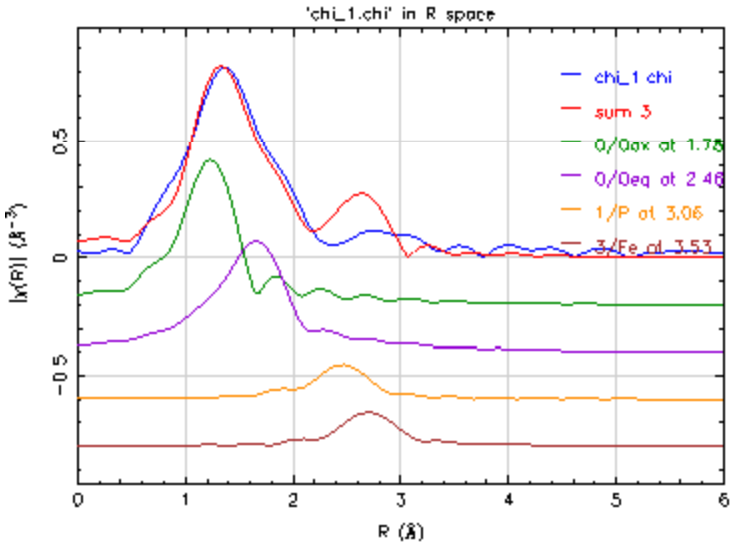


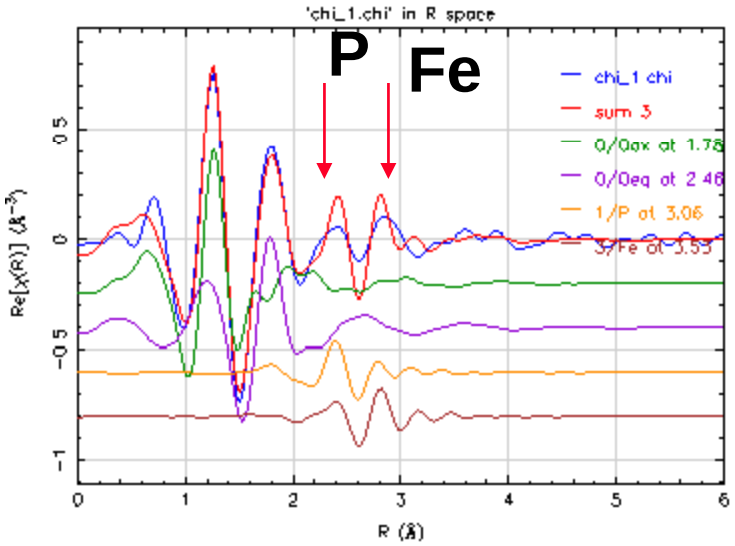

```
guess parameters:
  delE0          =  -7.20937844    # +/-   25.65700008     [0.65657]
  NO1            =   2.22860092    # +/-    4.20495043     [1.78168]
  NO2            =   6.33953720    # +/-   20.07574162     [4.50466]
  Nc             =  25.82138011    # +/-  165.30584186     [1.86426]
  delo1          =  -0.01877158    # +/-    0.08048129     [0.00291]
  delo2          =  -0.23126958    # +/-    0.12749206     [-0.18795]
  delc           =  -0.00779122    # +/-    0.20421510     [0.01691]
  sigo1          =  -0.00264827    # +/-    0.01911759     [4.54854e-006]
  sigo2          =   0.00862383    # +/-    0.03432931     [0.00466]
  sigc           =  -0.02507432    # +/-    0.09622080     [0.00410]
  Nfe2           =  34.92309218    # +/-  189.97303278     [1.54468]
  delfe2         =  -0.24162087    # +/-    0.31863129     [-0.17012]
  sigfe2         =   0.04511482    # +/-    0.09811547     [0.01153]
```

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

Signals became broad and unrealistic

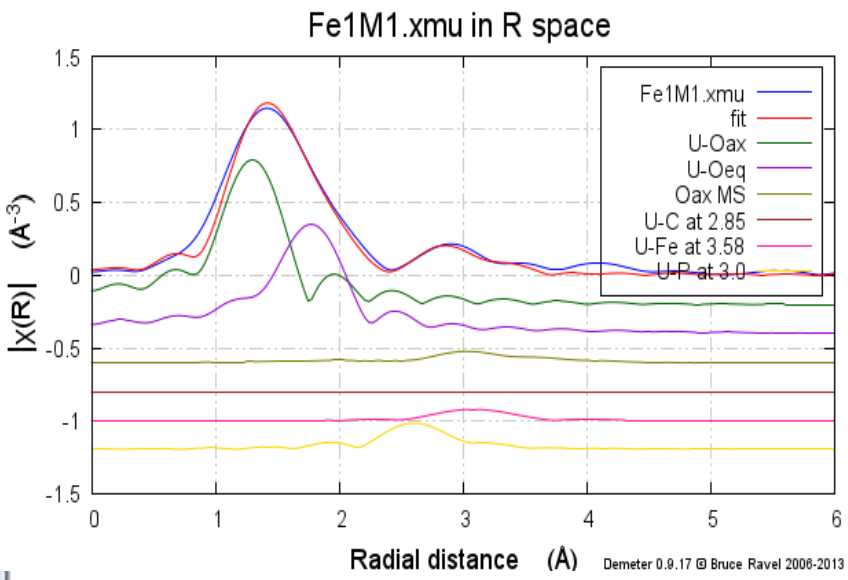
Test data for P and Fe shells

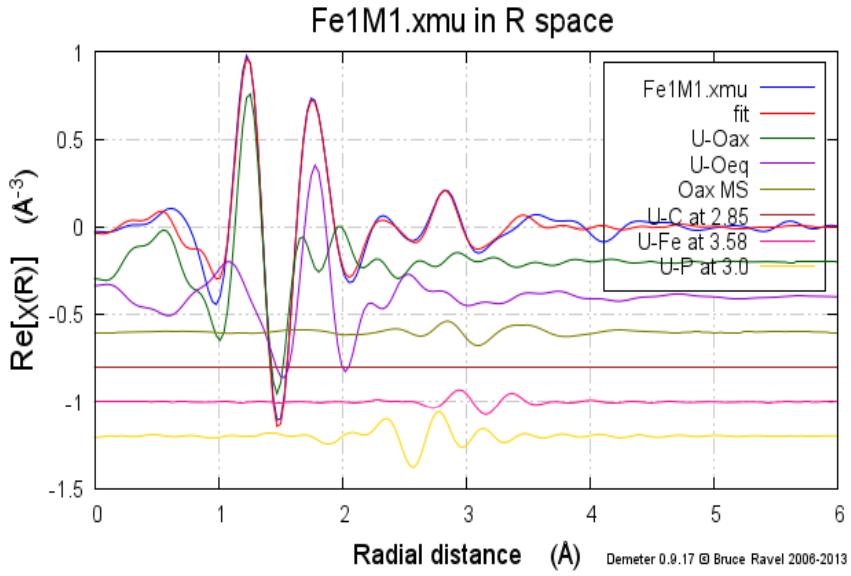




- **Place P and Fe shells in a "good" spot**
  - **set parameters – no fitting**
  - **monitor results and fit spectra**

Fit Results using P and Fe shells



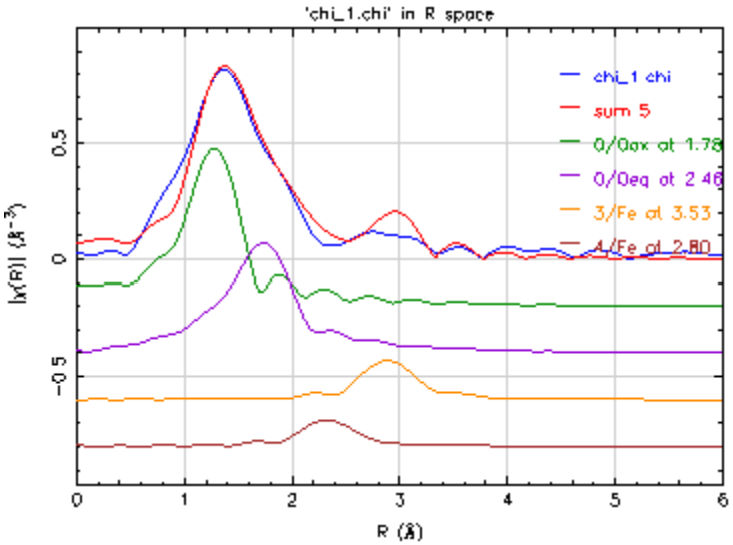


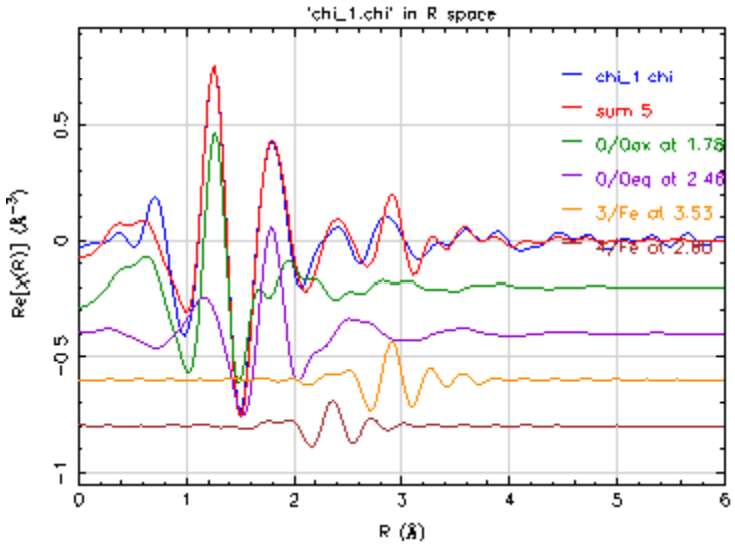

```
guess parameters:
  delE0          =    5.61401930    # +/-   27.80359821     [0.65657]
  NO1            =    1.87756022    # +/-    5.01084021     [1.78168]
  NO2            =    4.69820412    # +/-    8.94502263     [4.50466]
  delo1          =    0.02593456    # +/-    0.16855444     [0.00291]
  delo2          =   -0.15241235    # +/-    0.19664655     [-0.18795]
  sigo1          =    0.00000001    # +/-    0.02509008     [1.00742e-009]
  sigo2          =    0.00603437    # +/-    0.03047295     [0.00466]
  Nfe2           =    0.26864818    # +/-    7.34270113     [1.54468]
  delfe2         =   -0.05663159    # +/-    0.66187494     [-0.17012]
  sigfe2         =   -0.00036128    # +/-    0.22371051     [0.01153]
  delp1          =    0.07282056    # +/-    0.40898253     [0.06738]
  sigp1          =    0.00088094    # +/-    0.08136929     [0.00300]
  Np1            =    0.94722667    # +/-    7.57814884     [1.00000]
```

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

Signals became unrealistically sharp

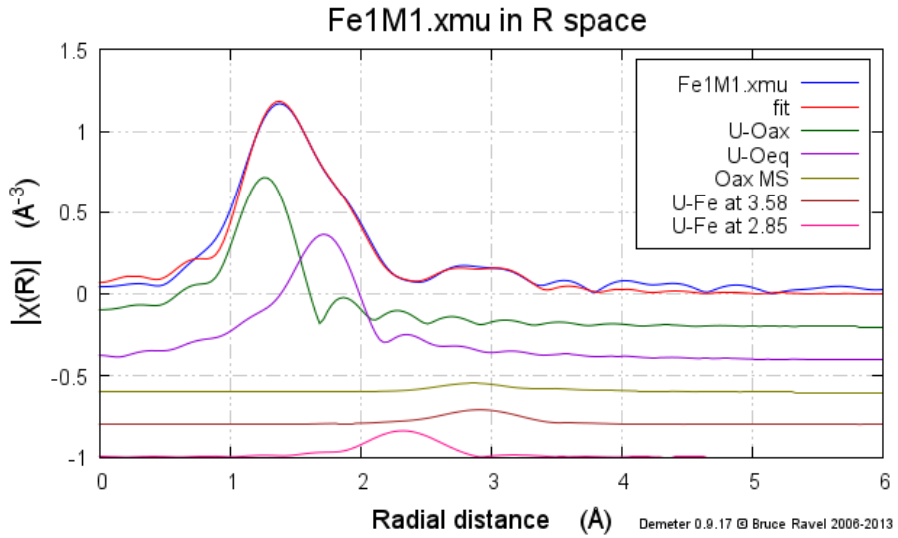
Test data for Fe and Fe shells

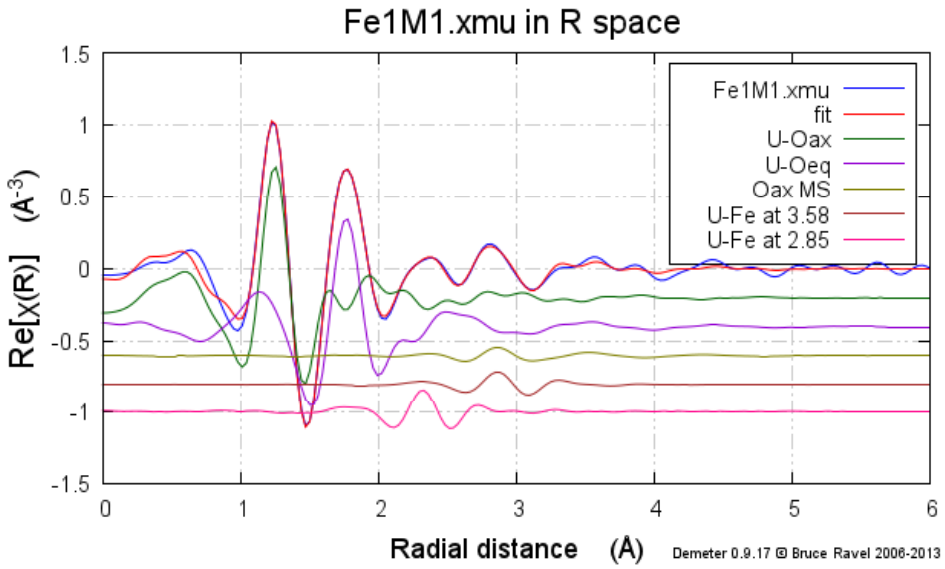




- **Place Fe and Fe shells in a "good" spot**
  - **set parameters – no fitting**
  - **monitor results and fit spectra**

Fit Results using Fe and Fe shells



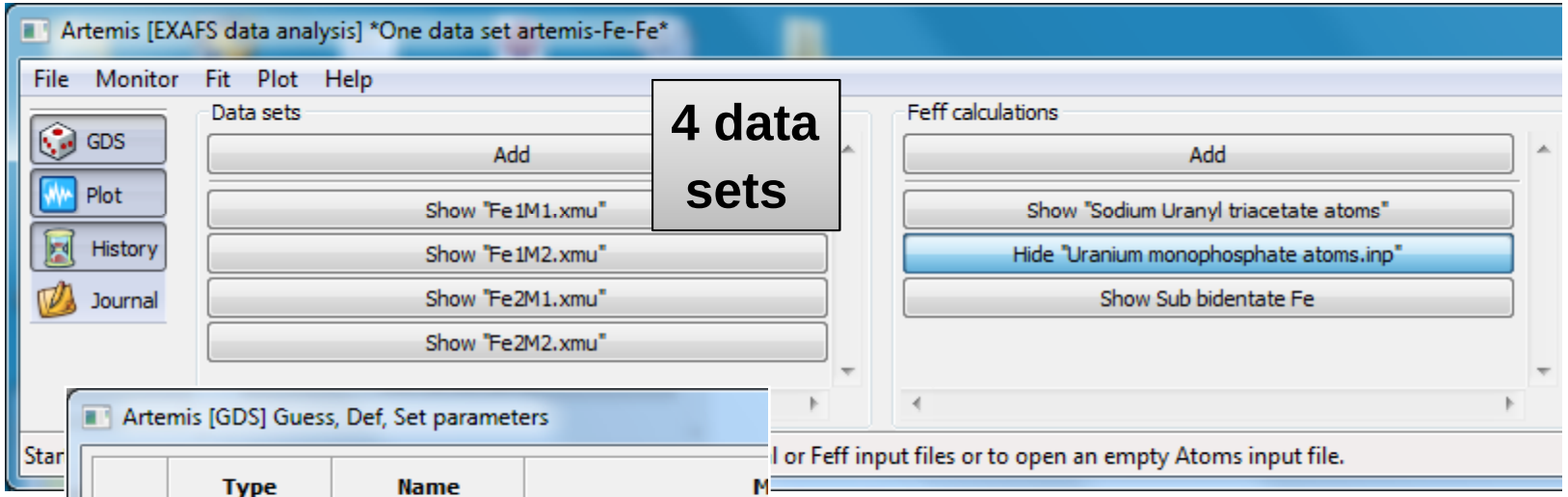


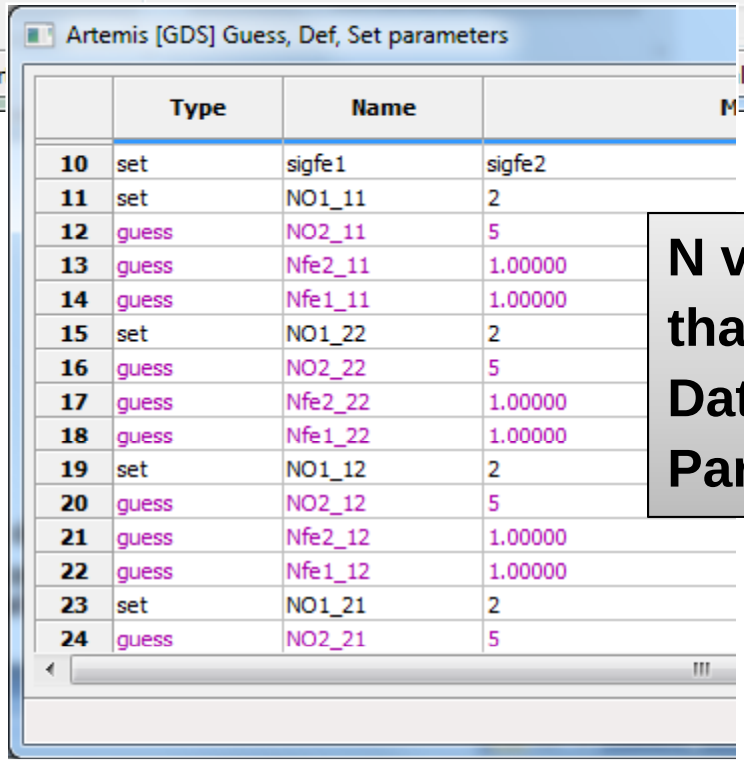

```
guess parameters:
  delE0              =  -0.52309493    # +/-   13.03833870     [5.57110]
  NO1                =   2.03134042    # +/-    1.61713414     [2.00000]
  NO2                =   5.73627907    # +/-    4.82822216     [3.96132]
  delo1              =   0.00417472    # +/-    0.05467323     [0.02440]
  delo2              =  -0.19840310    # +/-    0.07727996     [-0.15727]
  sigo1              =  -0.00170651    # +/-    0.00571344     [-0.00021]
  sigo2              =   0.00755140    # +/-    0.00688098     [0.00439]
  Nfe2               =   1.70423291    # +/-    6.96079514     [1.00000]
  delfe2             =  -0.16643599    # +/-    0.18133249     [-0.10000]
  sigfe2             =   0.01446017    # +/-    0.04156123     [0.00800]
  Nfe1               =   0.96716126    # +/-    0.84064342     [0.85186]
  delfe1             =  -0.01339862    # +/-    0.11102923     [0.05000]
```

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

Values are realistic, but uncertainties are large

Multiple data set fit





	Type	Name	M
10	set	sigfe1	sigfe2
11	set	NO1_11	2
12	guess	NO2_11	5
13	guess	Nfe2_11	1.00000
14	guess	Nfe1_11	1.00000
15	set	NO1_22	2
16	guess	NO2_22	5
17	guess	Nfe2_22	1.00000
18	guess	Nfe1_22	1.00000
19	set	NO1_12	2
20	guess	NO2_12	5
21	guess	Nfe2_12	1.00000
22	guess	Nfe1_12	1.00000
23	set	NO1_21	2
24	guess	NO2_21	5

N values that depend on Data set. All other Parameters are the same

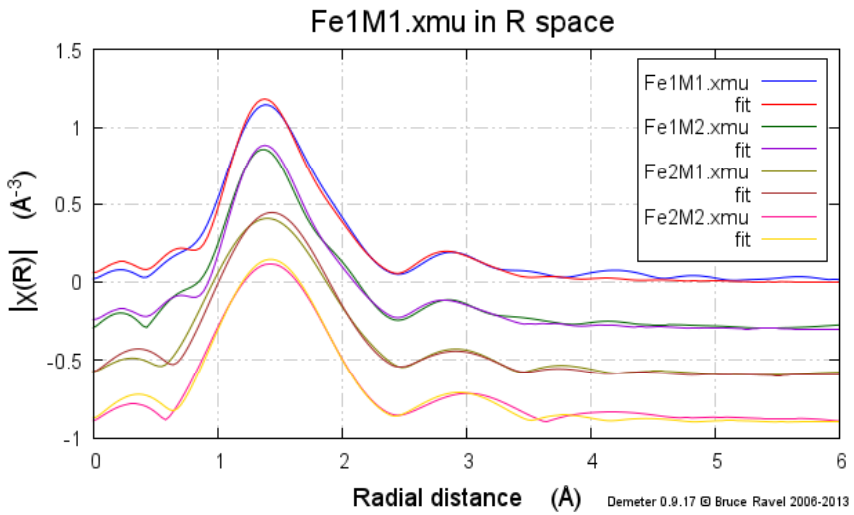
- **Fit 4 data sets**
- **Use K-weights of 1, 2 and 3**
- **Fit different N values for each data set**
- **Data series is needed to accurately determine the number of Fe atoms in the 2nd and 3rd shells**

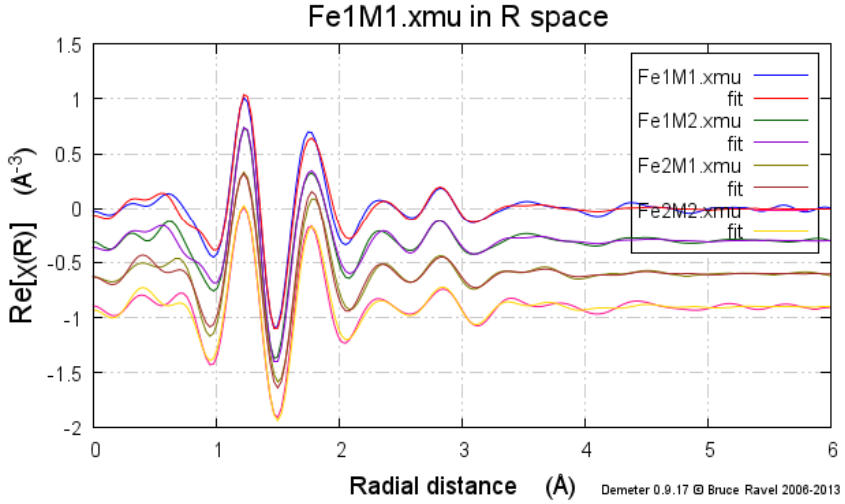
Modeling a Data Series

```
Independent points           : 29.7500000
Number of variables          : 11
Chi-square                   : 6548.0320163
Reduced chi-square           : 349.2283742
R-factor                     : 0.0455832
Measurement uncertainty (k)  : 0.0002134
Measurement uncertainty (R)  : 0.0003845
Number of data sets          : 4


Happiness = 74.42/100              color = #FEC182
   An R-factor of 0.04558 gives a penalty of 25.58320.
***** Note: happiness is a semantic parameter and should *****
*****    NEVER be reported in a publication -- NEVER!    *****

guess parameters:
  delfe2              =  -0.12831700    # +/-    0.01601433     [-0.12072]
  delfe1              =   0.01289046    # +/-    0.00693226     [0.01120]
  sigfe1              =   0.00647446    # +/-    0.00292661     [0.00611]
  Nfe2_11             =   0.66241492    # +/-    0.23026024     [1.10762]
  Nfe1_11             =   0.88582314    # +/-    0.34515786     [0.88654]
  Nfe2_12             =   0.53389948    # +/-    0.27788274     [0.92843]
  Nfe1_12             =   0.98037888    # +/-    0.38456367     [0.90765]
  Nfe1_21             =   1.17116425    # +/-    0.43261640     [1.01045]
  Nfe2_21             =   0.32360733    # +/-    0.29454535     [0.56411]
  Nfe2_22             =   0.67699484    # +/-    0.34524740     [1.20824]
  Nfe1_22             =   0.99083810    # +/-    0.39030744     [0.92682]
```





Reasonable modeling of data series

Summary

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- **Athena and Artemis: a complete set of tools to process XAS spectra utilizing Ifeffit.**
- **Thank-you to the authors Bruce Ravel (A&A) and Matt Newville (Ifeffit).**
- **When you get stuck, check out the ifeffit mailing list for help from the experts: http://cars9.uchicago.edu/mailman/listinfo/ifeffit/**