

Feff7.exe and feff7.bat copied in the default directory



C:\Program Files\Ifeffit\feff7.bat

```
1 @echo off
2 SET IFEFFIT_DIR=C:\Program Files\Ifeffit
3 SET PATH=%PATH%;%IFEFFIT_DIR%
4 SET PGPLOT_DIR=%IFEFFIT_DIR%
5 SET PGPLOT_DEV=/GW
6 cd "%IFEFFIT_DIR%"
7 "%IFEFFIT_DIR%\runprog.exe feff7
8
```

I edited feff6l.bat and renamed it feff7.bat

Current project: modified

Edit Preferences

- All parameters
- general
 - geometry
 - plot
 - data
 - log
 - gds
 - athena
 - atoms
 - feff
 - feff_exec
 - autoparams
 - intrp
 - paths
 - warnings
 - logview
 - histogram
 - colors
 - fonts

Parameter: feff_executable
 Type: string
 Artemis' Default: feff6l
 Value: feff7

Description

This variable gives the name of the Feff executable.

Press the "Default" button to restore Artemis' default value for this variable.

Set ALL parameters to Artemis' defaults

Apply changes to this session

Save changes for future sessions

Return to the main window

Data & Paths

Guess, Def, Set

- FE00AL.ak0
- FEFF0

Fit

k R q

Plotting options

0 1 2 3 kw

Main Indic Traces

Plot in R: Magnitude
 Real part
 Imaginary part

Plot in q: Magnitude
 Real part
 Imaginary part

Window
 Background
 Residual

kmin: 2	kmax: 15
Rmin: 0	Rmax: 6
qmin: 0	qmax: 15

Document: Plotting

Current project:

modified

Atoms feff.inp Interpretation

```

* specific gravity = 4.200
* ---*---*---*---*---*---*---*---*---*---*---*---*---*---*---*
* Normalization correction: 0.00061 ang^2
* ---*---*---*---*---*---*---*---*---*---*---*---*---*---*---*
*
* The following crystallographic data were used:
*
* title          Goethite
* space = P n m a
* a = 4.61580    b = 9.95450    c = 3.
* alpha = 90.0  beta = 90.0  gamma = 90.0
* core = Fe      edge = K
* atoms
* ! elem  x      y      z      tag      occ
* Fe     0.04790  0.85420  0.75000  Fe      1.00
* O      0.70800  0.19880  0.75000  O1      1.00
* O      0.19700  0.05270  0.75000  O2      1.00
*
*
* TITLE Goethite
*
* HOLE 1 1.0 * Fe K edge (7112.0 eV), second number is
*
* mphase,mpath,mfeff,mchi
* CONTROL 1 1 1 1
* PRINT 1 0 0 3
*
* RMAX 10.0
    
```

Data & Paths

- Guess, Def, Set
- [-] FE00AL.ak0
- [-] FEFF0

Fit

k R q

Plotting options

0
 1
 2
 3
 kw

Main Indic Traces

- Plot in R: Magnitude
- Real part
- Imaginary part
- Plot in q: Magnitude
- Real part
- Imaginary part

Window

Background

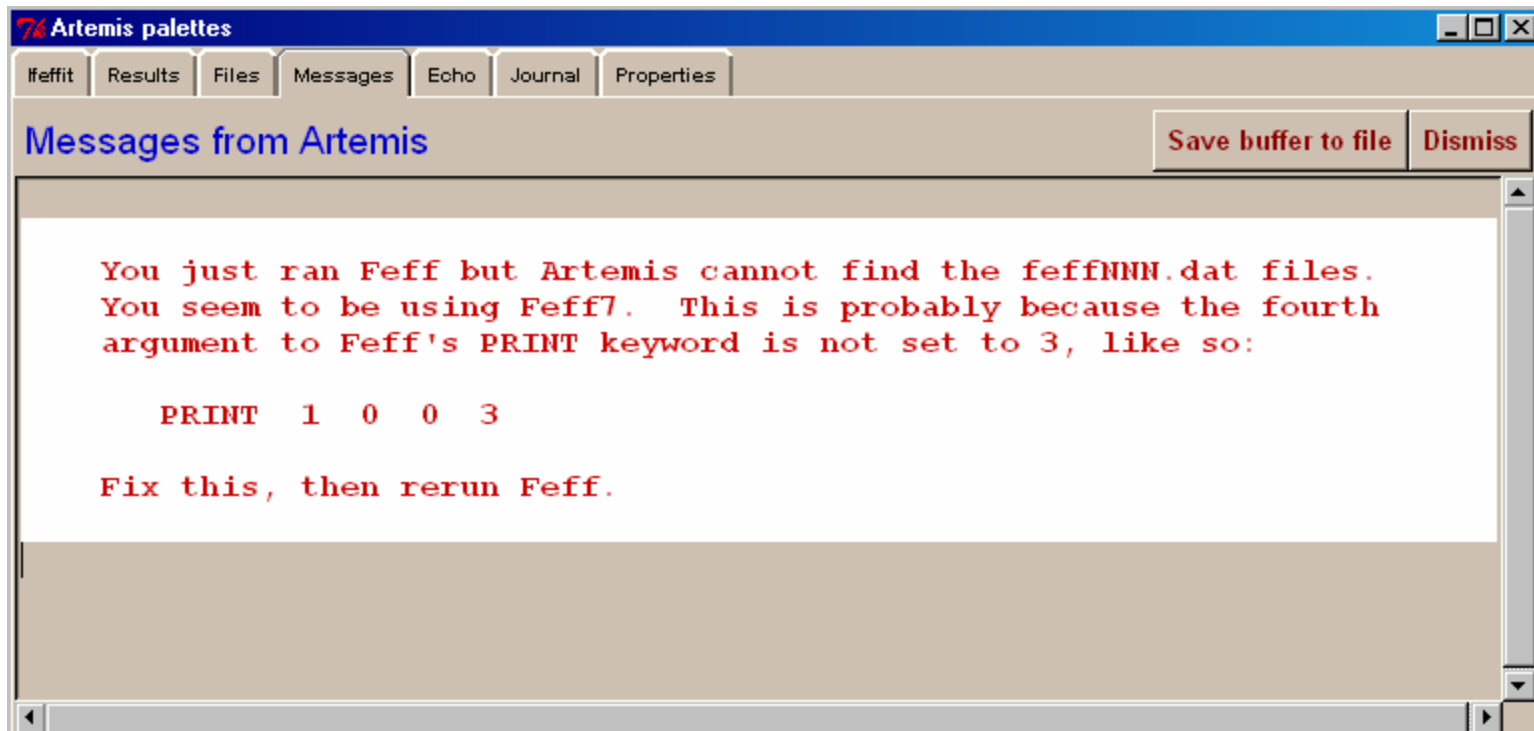
Residual

kmin: 2	kmax: 15
Rmin: 0	Rmax: 6
qmin: 0	qmax: 15

Run Feff
Document: Feff and it's input file

Document: Plotting

Here is the erreur message I obtain:



Next is a rather minor question.....

Although the k-range for the fit is prescribed between 2.4 and 14.3 A-1.....

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

- Current project:** FE00AL.ak0 (modified)
- Data & Paths:** A tree view showing the data file FE00AL.ak0 and its paths (Path 1 to Path 22).
- Fit Parameters:**
 - Data controls:** Include in the fit, Plot after the fit, Fit background
 - Fourier and fit parameters:** k-range [2.429, 14.311], R-range [0.730, 9.553], dk [2], dr [0.1], k window [Kaiser-Bessel], R window [Kaiser-Bessel]
 - Other parameters:** Fitting space [k], Epsilon [0], Minimum reported correlation [0.25], Path to use for phase corrections [None]
 - Fit k-weights:** kW=1, kW=2, kW=3, other k weight
- Plotting options:**
 - Plot in R:** Magnitude, Real part, Imaginary part
 - Plot in q:** Magnitude, Real part, Imaginary part
 - Window, Background, Residual
 - Axis ranges:** kmin: 2, kmax: 15; Rmin: 0, Rmax: 10; qmin: 0, qmax: 15

66 independent points data points (Nyquist): (1 data set) (5 variables)

The plot limits are different.....

