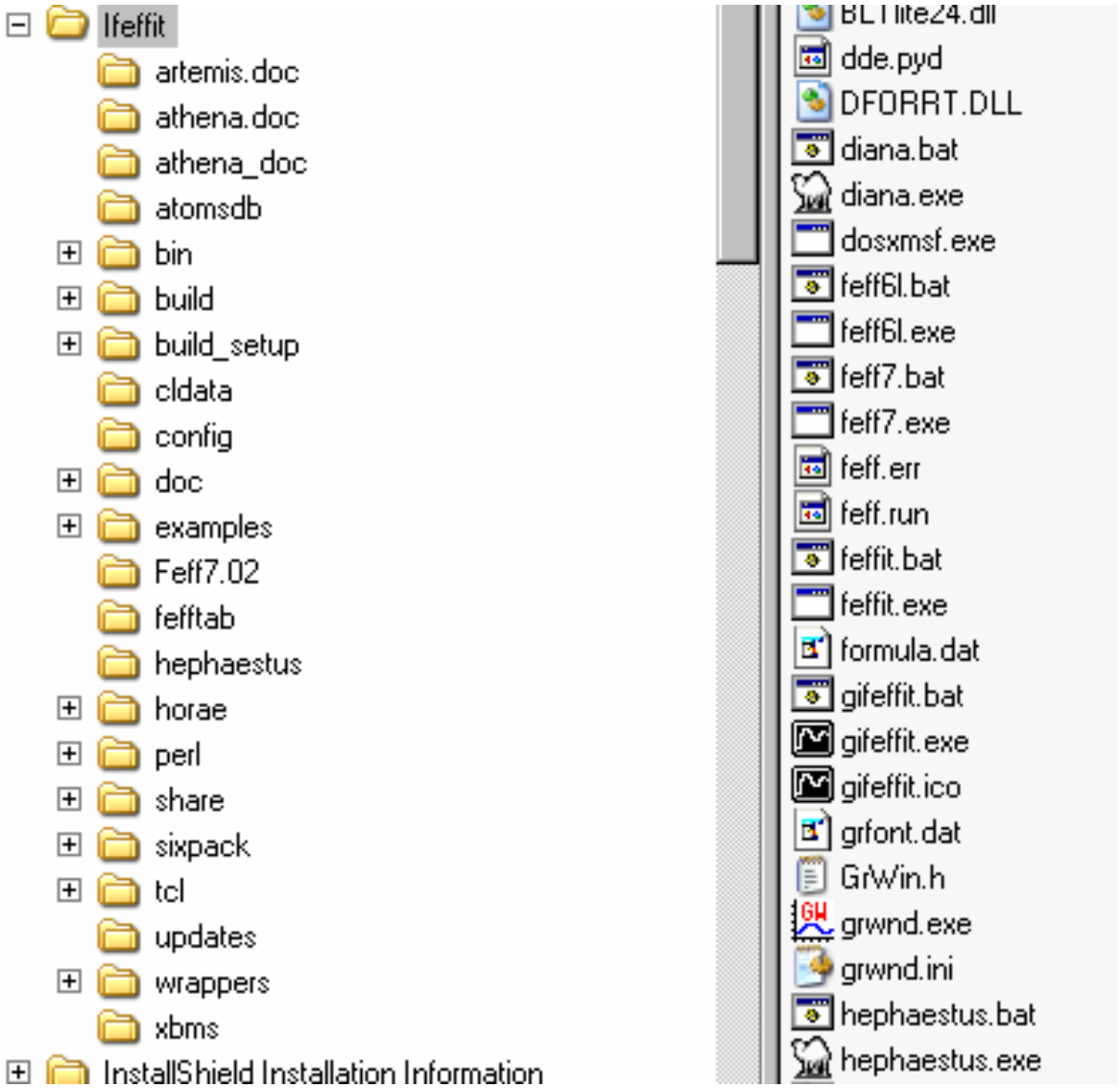
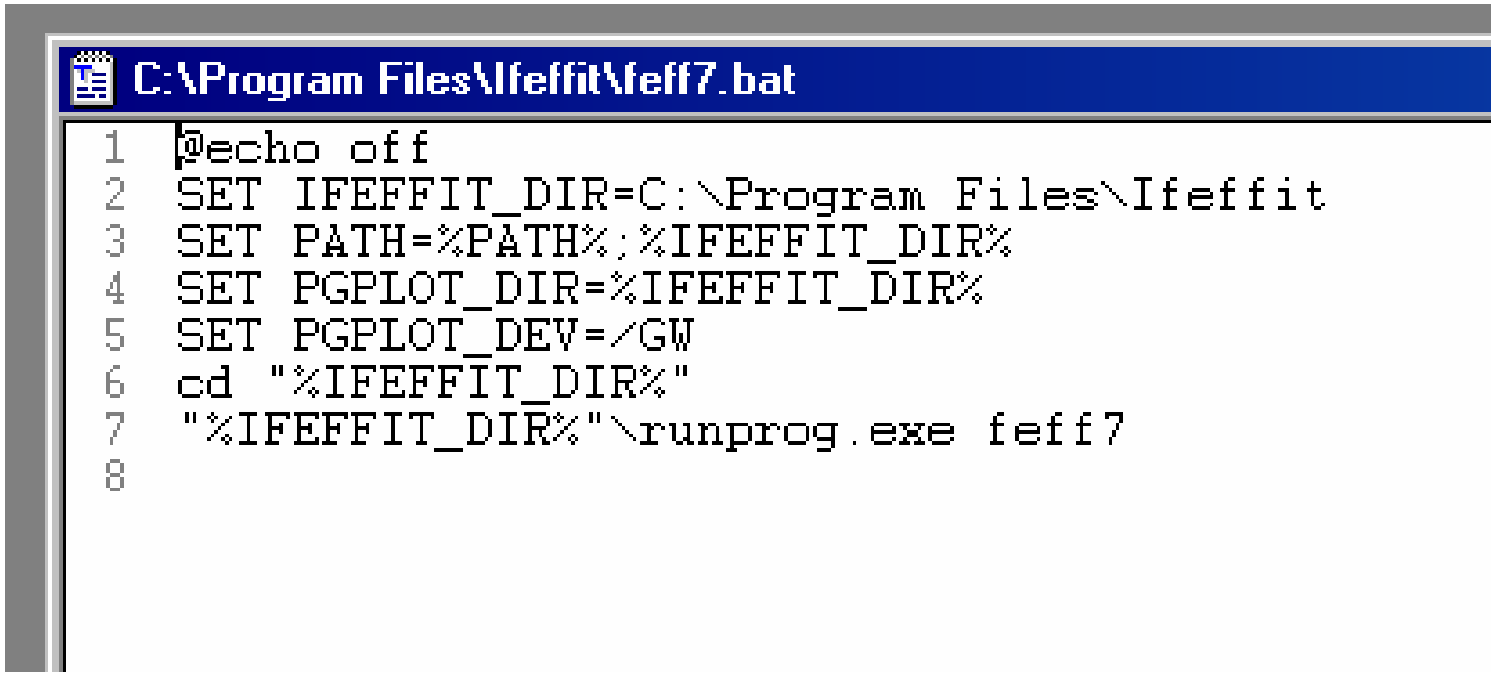
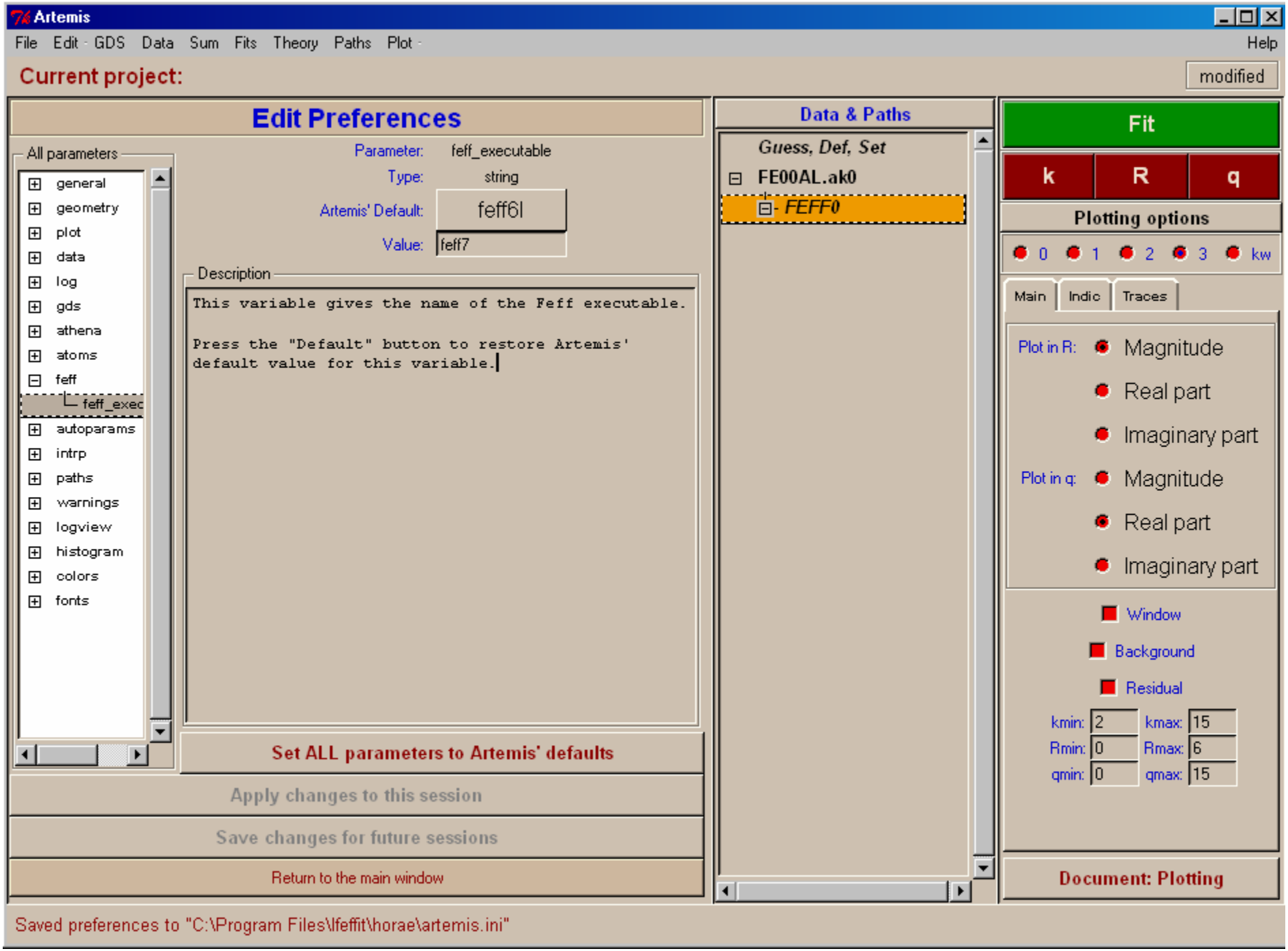
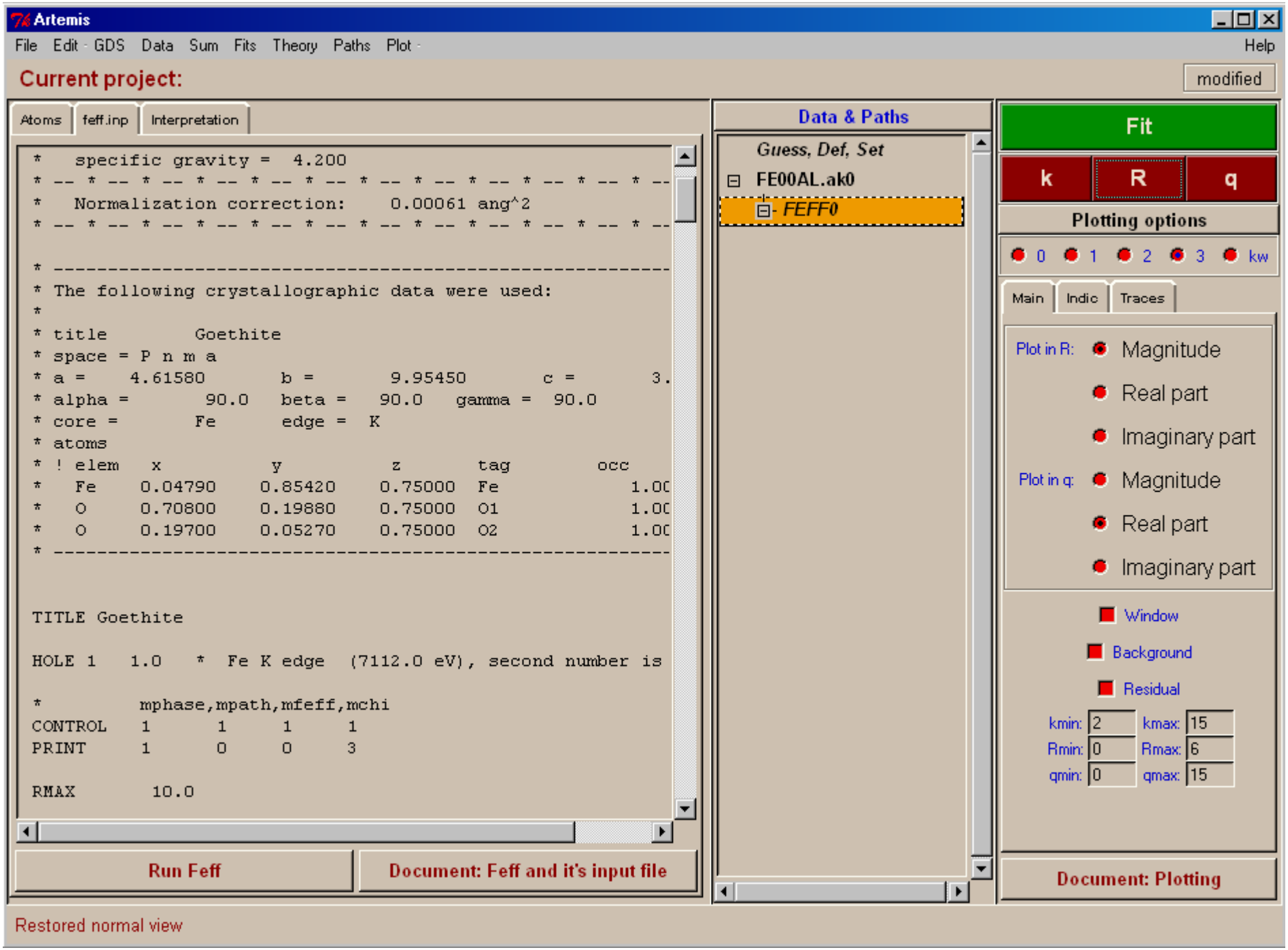


Feff7.exe and feff7.bat copied in the default directory

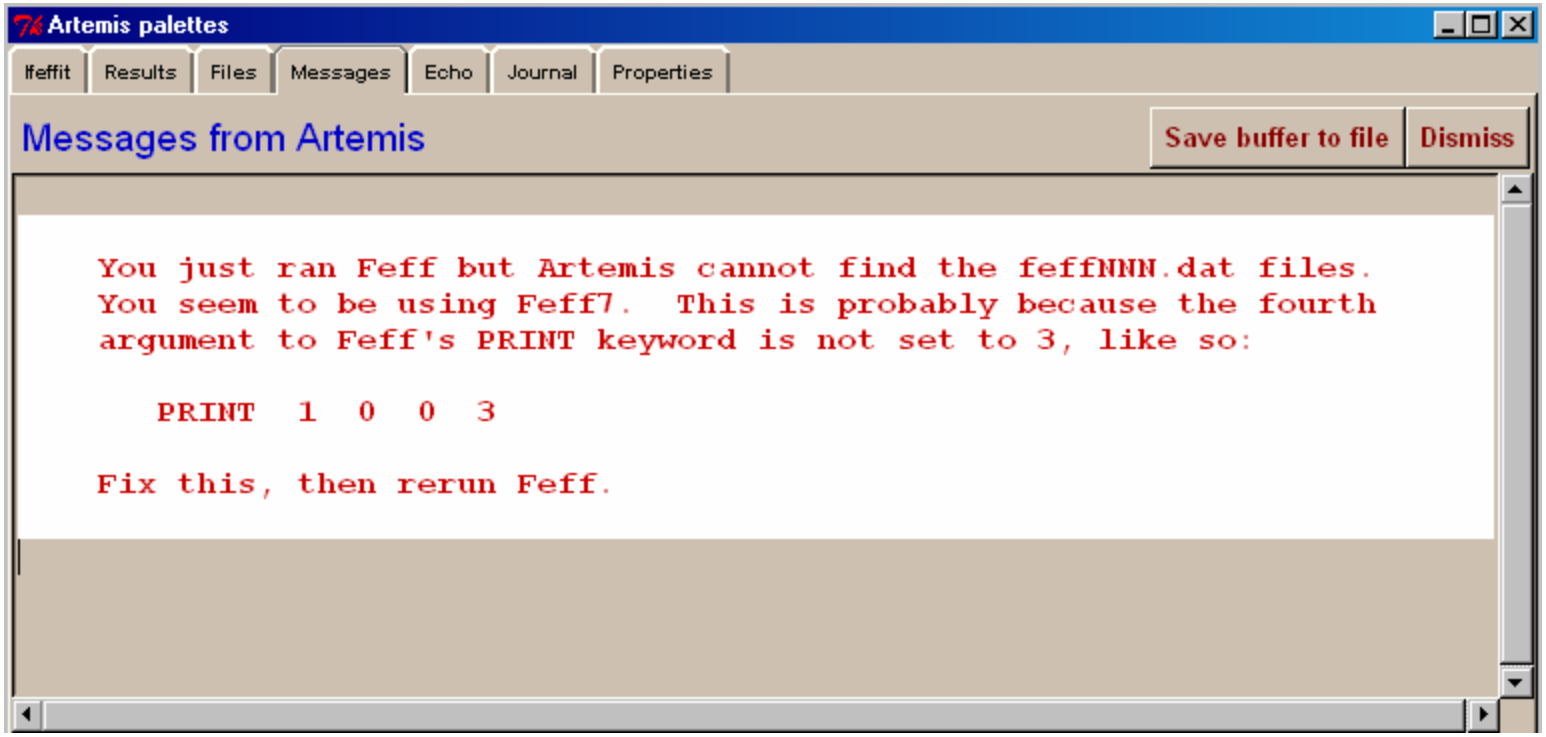


I edited feff6l.bat and renamed it feff7.bat


Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
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
Saved preferences to "C:\Program Files\lfeffit\horae\artemis.ini"

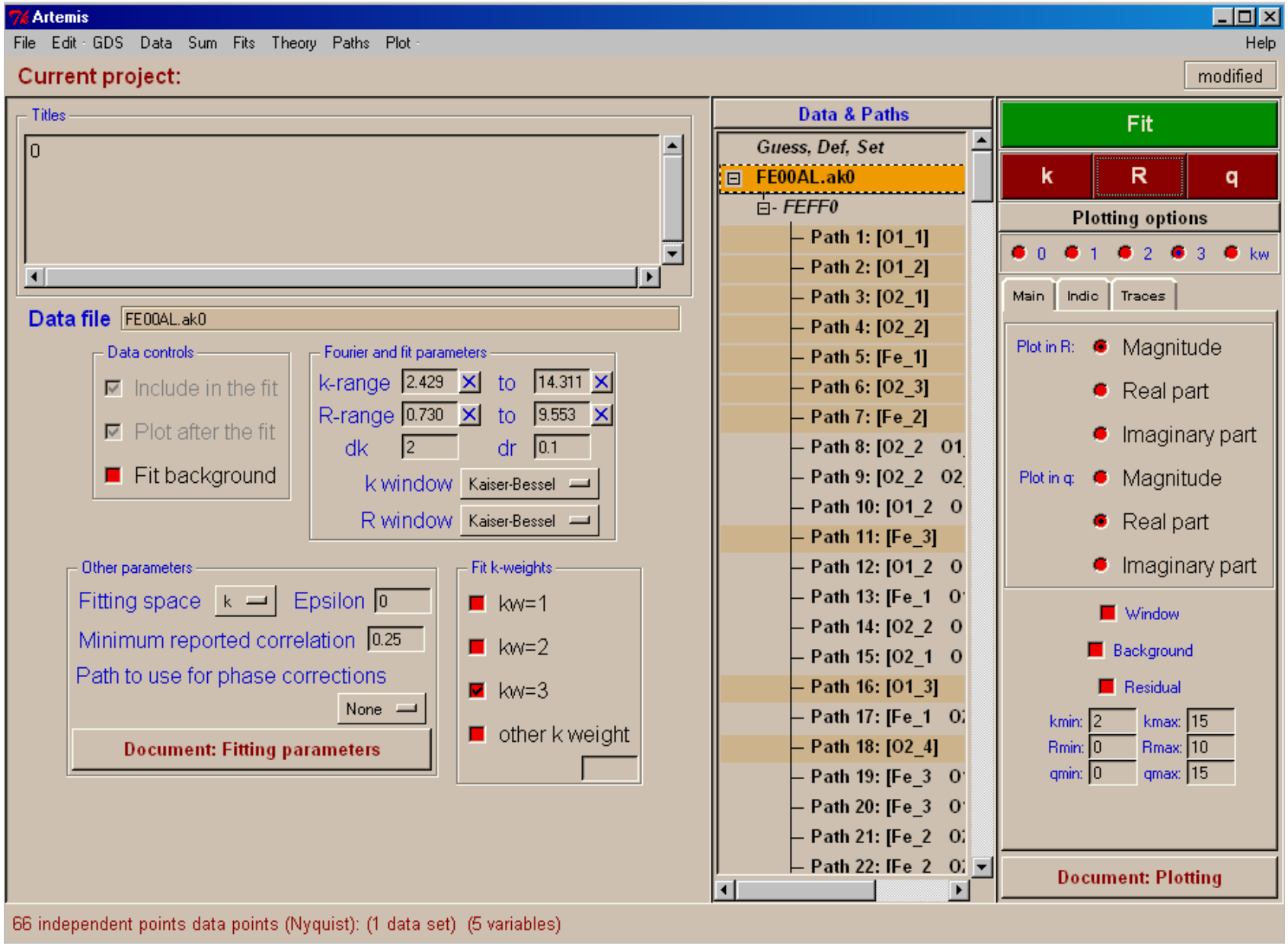

Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
Current project:
modified
Atoms feff.inp Interpretation
* specific gravity = 4.200
* Normalization correction: 0.00061 ang^2
* The following crystallographic data were used:
* title Goethite
* space = P n m a
* a = 4.61580 b = 9.95450 c = 3.
* 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 1.0
* O 0.70800 0.19880 0.75000 O1 1.0
* O 0.19700 0.05270 0.75000 O2 1.0
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
Run Feff
Document: Feff and it's input file
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
Restored normal view

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 plot limits are different…..