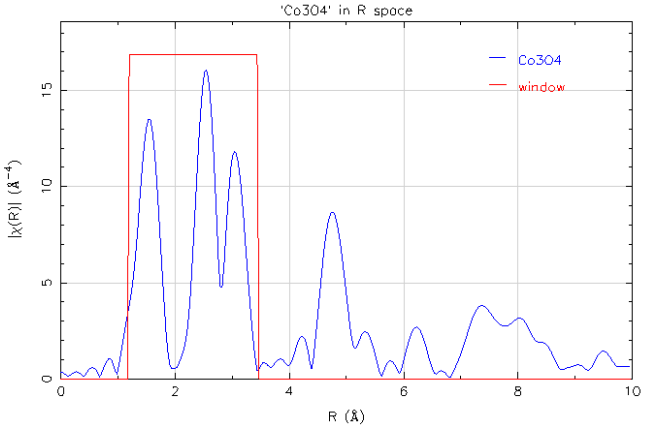
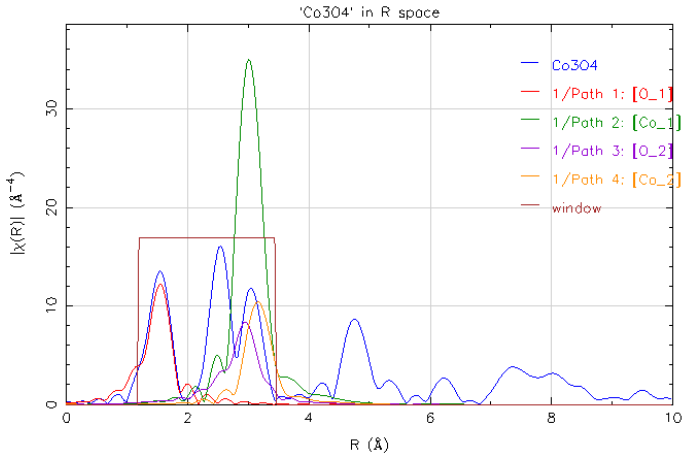
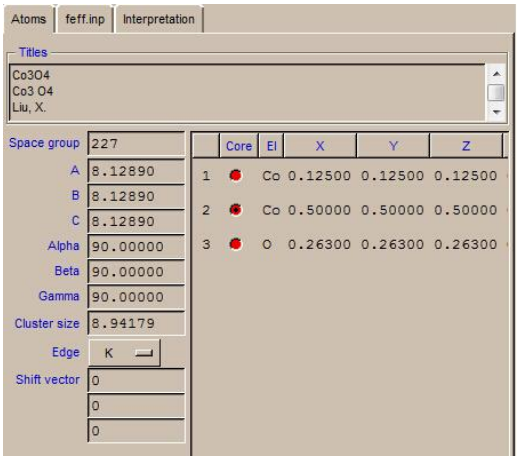
Experimental:



Model (Co3O4, space group: #227):






```
"F d -3 m" appears in the International Tables with
multiple choices of origin.  If the atoms list seems wrong, you
should use a shift vector of:
      -0.125, -0.125, -0.125
```

Questions:

(1) Why the second peak (ca. 3 Å) in experimental data is missing in the Co3O4 model?

(2) Why need to add the “shift vector” suggested by Artemis? Actually, no action is required and the software change the Co core from 0.125, 0.125, 0.125 to 0.5 0.5 0.5, and keep the shift vector as 0 0 0.