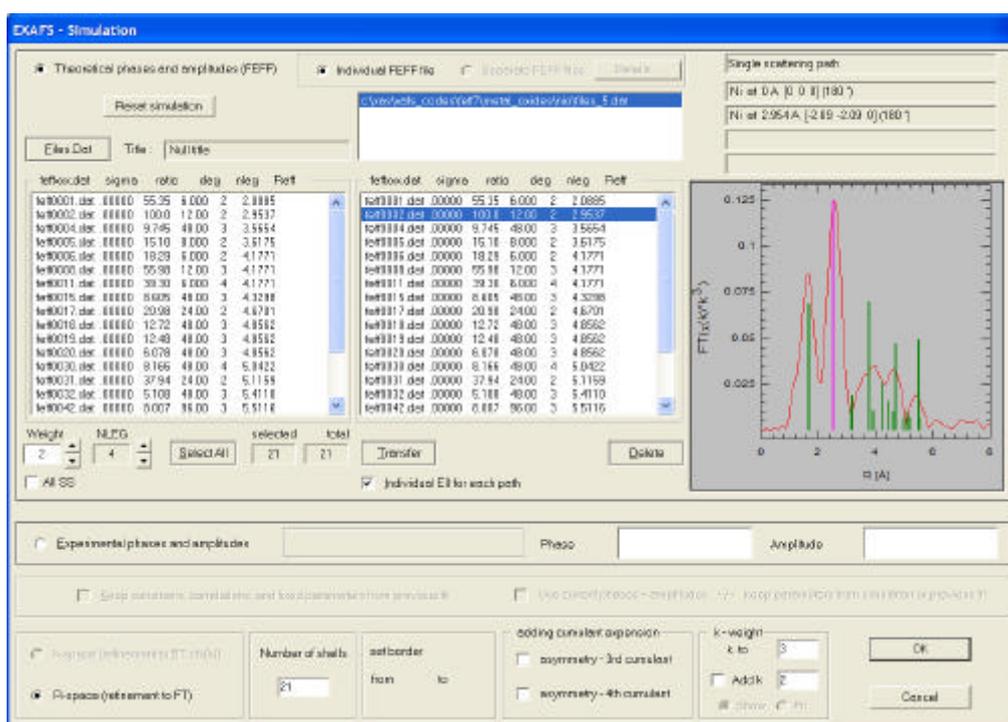


New features in WinXAS version 3.1

(released 03/04)

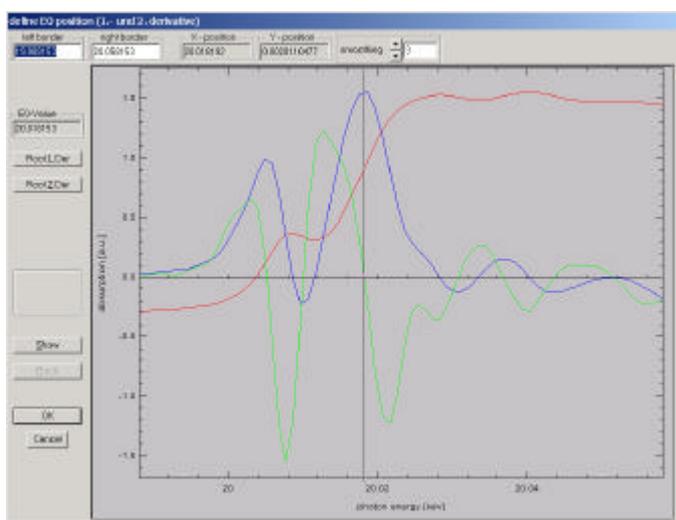
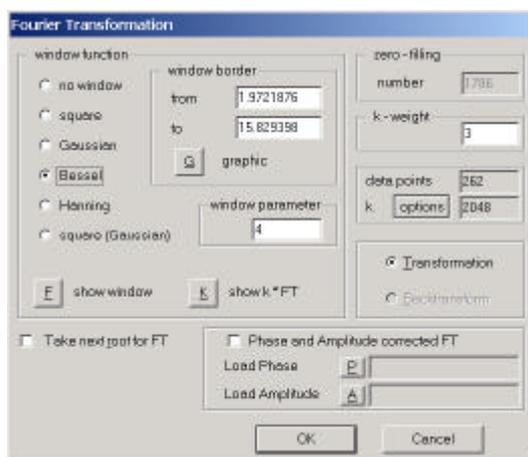
The interface to FEFF has been improved in terms of (i) selection of paths from different calculations, (ii) graphical display of the paths selected, (iii) display of coordinates of individual paths, etc.



New features in WinXAS version 3.0

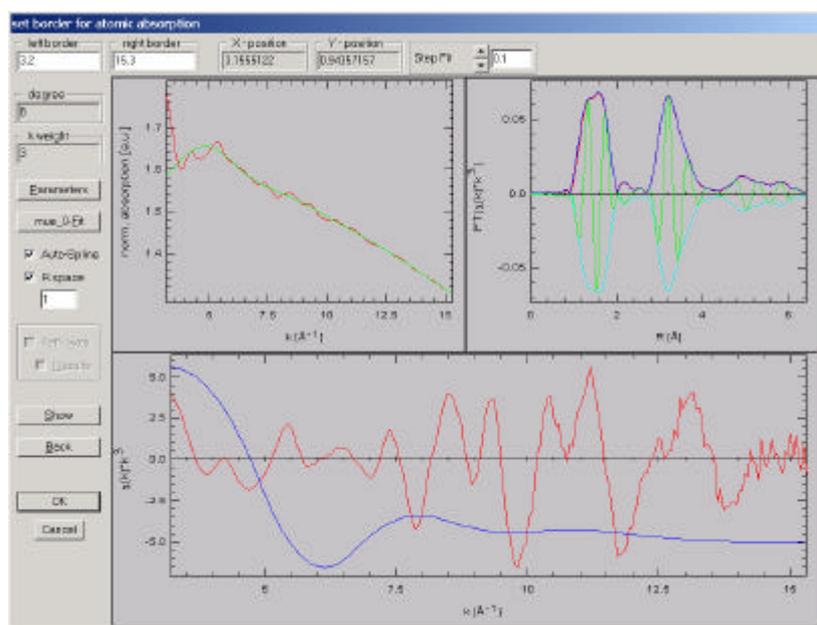
(released 12/03)

1) In many dialog boxes the parameters are saved and displayed next time (for instance in the Fourier transform dialog box)

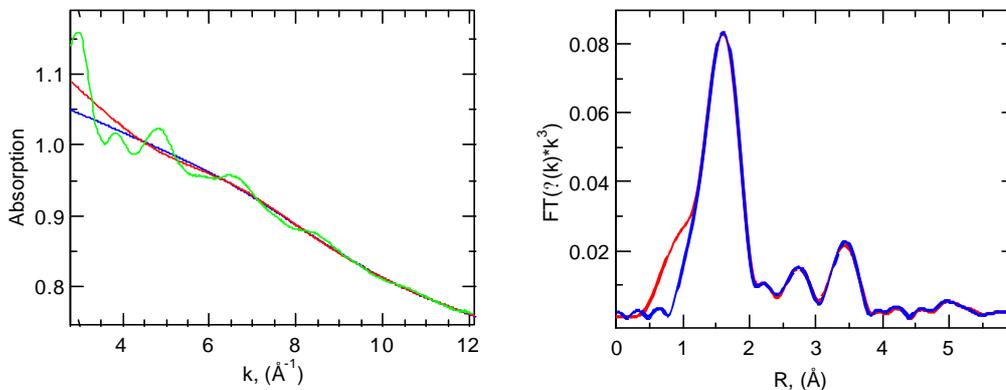


2) For energy calibration and sample E_0 determination suitable starting parameters for the fitting range and the E_0 parameter are pre-determined automatically and displayed.

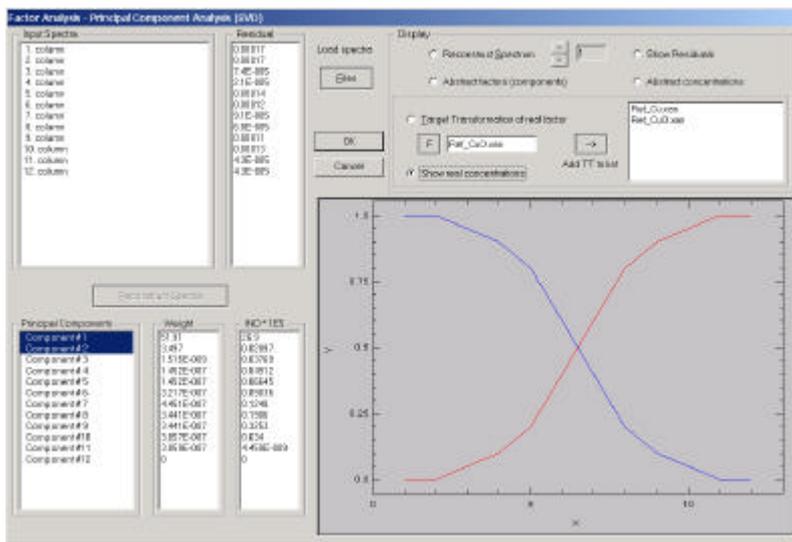
3) For the $\mu(0)$ refinement (atomic absorption), a suitable number of spline knots is calculated from $N(\text{spline})=2/\text{PI}*\text{dk}*dR+1$ (i.e. “Auto spline” option). During the refinement procedure, the number of spline is readjusted according to the chosen range in k space (dk) and the “fitting” range in



R space (dR). Furthermore, the $\mu(0)$ refinement can be performed in the R space to minimize the amplitude in the $FT(\chi(k))$ at $R < dR$. This results in a much improved and more stable $\mu(0)$ refinement (Figures), while providing a maximum of transparency and control of the underlying procedures.



4) The Factor Analysis (Principal component analysis) dialog box permits the calculation of real factors (e.g. chemical species) from reconstructed spectra and target transformed references. This is an alternative procedure that offers several advantages compared to using a least-squares refinement of selected references (LC XANES fit).



5) The XAFS refinement features an optional display of the experimental and theoretical $\chi(k)$ in addition to the $FT(\chi(k))$. Moreover, the refinement can be easily performed to differently weighted Fourier transformed $\chi(k)$ (e.g. simultaneous refinement to $FT(\chi(k)*k^1)$ and $FT(\chi(k)*k^3)$). The latter can result in more stable converging

