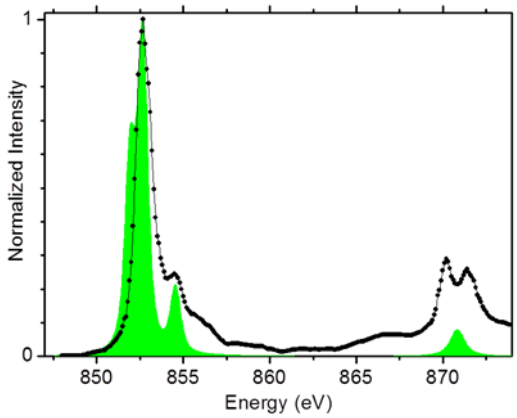
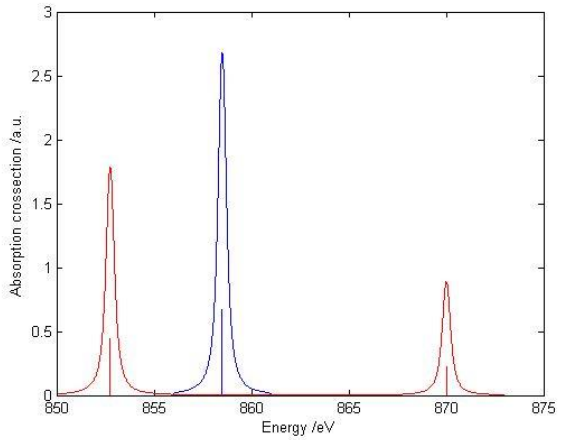
CTM4XAS: Discussion of tutorial exercises

Exercise 5: atomic multiplet spectrum of Ni2+



a) Calculate the atomic multiplet spectrum of Ni2+.
Set all parameters to zero. Plot the spectra with sticks on.

b) Set the 2p spin-orbit coupling to 1.0. Repeat the calculation. Explain the spectrum.

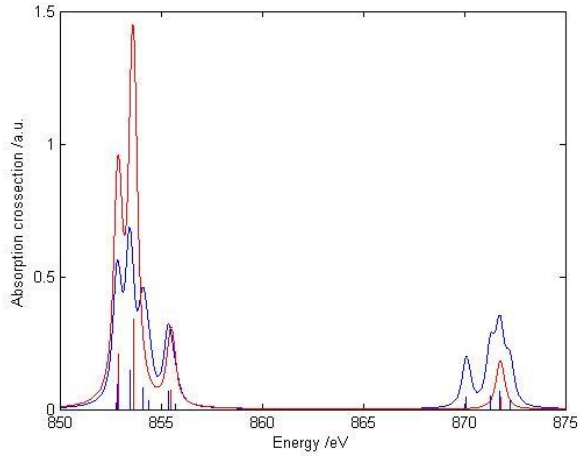


The blue spectrum has all atomic values set to zero. There is 1 peak related to the binding energy of the 2p core state.

The red spectrum has the 2p spin-orbit switched on. There are two peaks with a ratio 2:1, following the degeneracy of the 2p3/2 and 2p1/2 states.

c) Set the Slater integrals to 1.0. Repeat the calculation. Explain the spectrum.

d) Set the 3d spin-orbit coupling to 1.0. Repeat the calculation. Explain the spectrum. Why are some sticks missing in comparison with calculation c).



The blue spectrum (4c) has the Slater integrals on but the 3d spin-orbit coupling set to zero.

The red spectrum (4d) has the 3d spin-orbit coupling switched on.

Some peaks are not present in the red spectrum. The reason is that the 3d spin-orbit coupling creates an energy difference between the 3F states and only the 3F4 state is occupied. From 3F4 only final states with J=3, 4 or 5 Without 3d spin-orbit coupling also the 3F3 and 3F2 states are occupied and states with J=2 and J=1 can also be reached.

e) Why does the calculation not look like the 2p XAS spectrum of NiO yet?
Because the crystal field is not included.