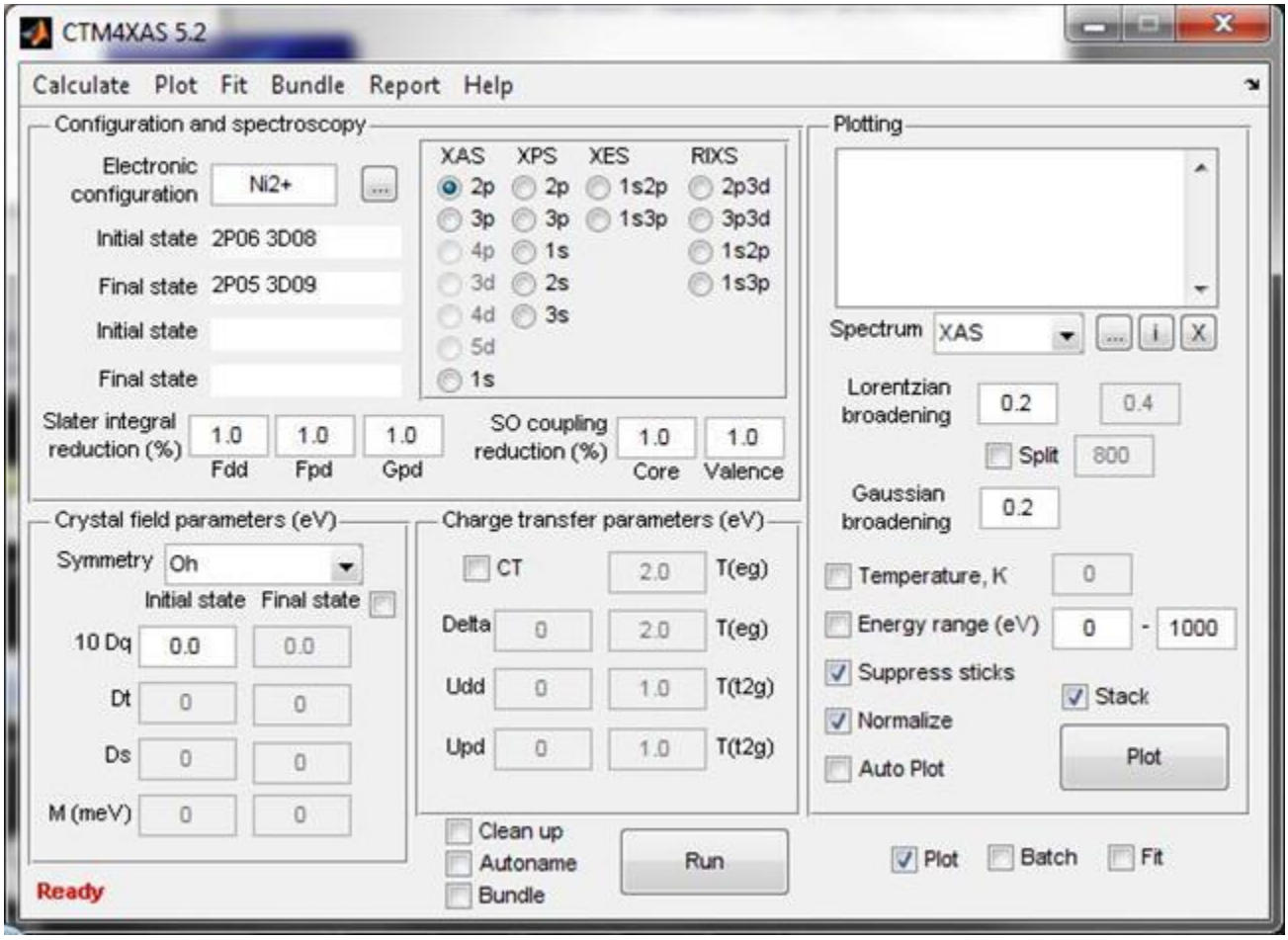
CTM4XAS: Discussion of tutorial exercises

Exercise 1: A first calculation with the CTM4XAS interface

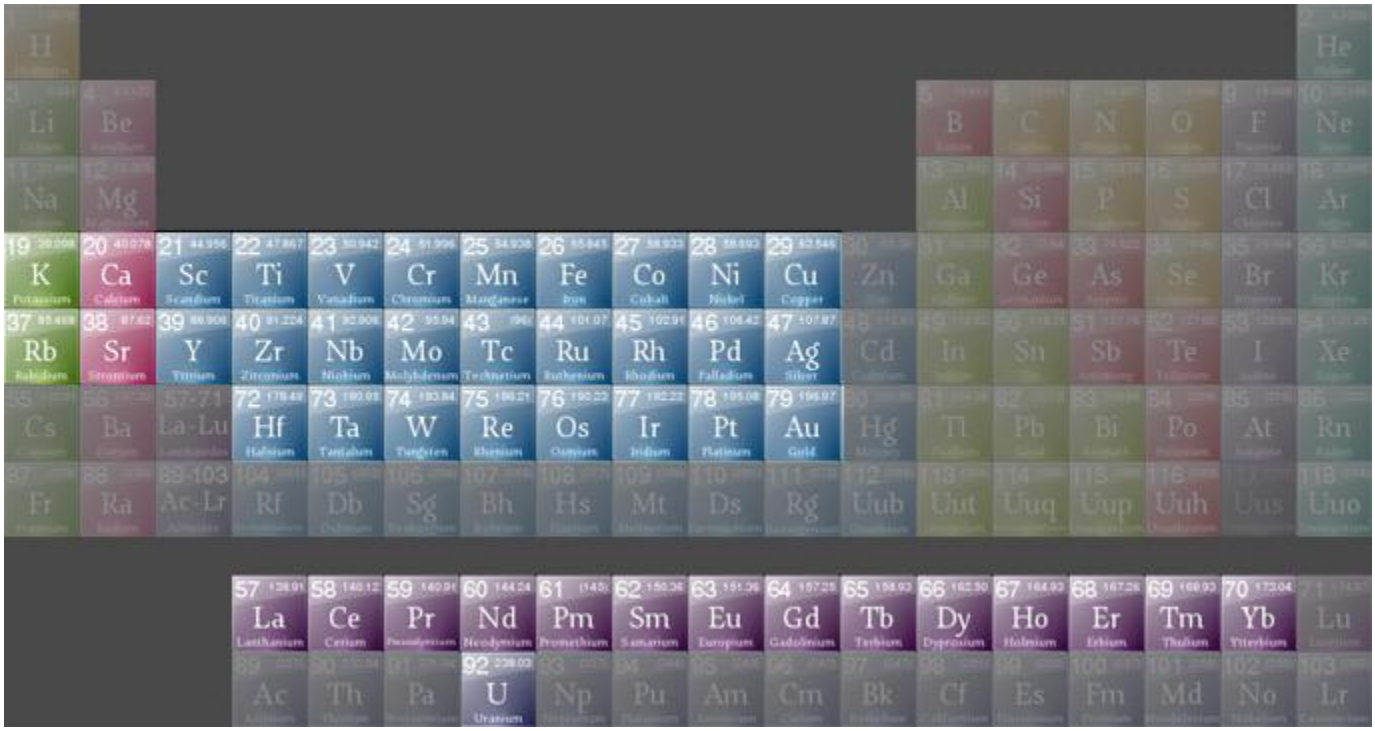
In the first calculation with the CTM4XAS interface we calculate the atomic multiplet spectrum of Ti4+, where the focus is on the practical aspects of the interface.

a) Start the CTM4XAS55.exe file (55 is the version number).
The CTM4XAS window opens (the figure shows version 5.2).



b) Select the □ button before “Auto Plot”.
This tells the interface to directly show the spectrum on the screen when it is calculated.

c) Press the □ button behind “Ni2+”.
This open a new window with the periodic table.



d) Select Ti.
This opens a new window with the optional valences. Choose 4+.

e) You now return to the CTM4XAS window and press the RUN button.
A window opens that asks for a filename. Choose ti4 as filename.
Now the calculation starts and after max. 30 seconds a new window with the Ti4+ spectrum.

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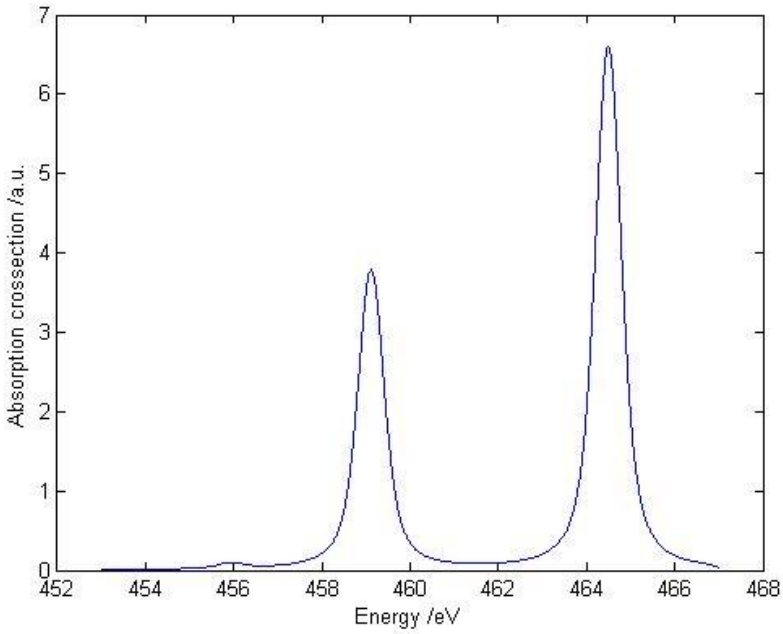

This is the atomic multiplet spectrum of Ti4+. You can remove the sticks by selecting the □ button before "Suppress sticks" and then select the PLOT button.

f) Look into the directory from which you started CTM4XAS55.exe.
Order the files by date and search for all file with the name ti4.

You find the files ti4.xy, ti4.nfo, ti4.rcg, ti4.rac, ti4.ora, ti4.plo, ti4.org and ti4.param

1. The file ti4.xy contains 4 columns with numbers, respectively the energy, the absorption for left polarized x-rays, the absorption for right polarised x-rays and the absorption for z-polarised x-rays. The XAS spectrum is the addition of the three spectra, but for an atomic calculation the three columns are identical.
2. The file ti4.nfo contains all values of the parameters used.
3. The file ti4.rcg is the inputfile for the atomic multiplet calculation.
4. The file ti4.rac is the inputfile for the crystal field multiplet calculation.
5. The file ti4.ora is the outputfile for the crystal field multiplet calculation.
6. The file ti4.plo is the inputfile for the plot program.
7. The file ti4.org is the outputfile for the atomic multiplet calculation.
8. The file ti4.param is a Matlab- format file with the parameters.

If the calculation works well, you do not need to use files 3 to 8.