

## CTM4XAS: Tutorial exercises

### **Exercise 2: manipulating the atomic multiplet spectrum of Sc<sup>3+</sup>**

Explain in every step the (changes in the) spectral shape.

- a) Sc<sup>3+</sup> has a 3d<sup>0</sup> configuration. What is the ground state symmetry?
- b) What is the final state configuration in a 2p XAS experiment?
- c) How many peaks will be visible in the spectrum? Explain.
- d) Calculate the atomic multiplet spectrum of Sc<sup>3+</sup>, with the name sc3d.
- e) Set Fpd and Gpd to zero and repeat the calculation with the name sc3e.
- f) Set Fdd to zero and repeat the calculation with the name sc3f.
- g) Set the 2p spin-orbit parameters to zero (sc3g).
- h) Set the 3d spin-orbit coupling to zero (sc3h).