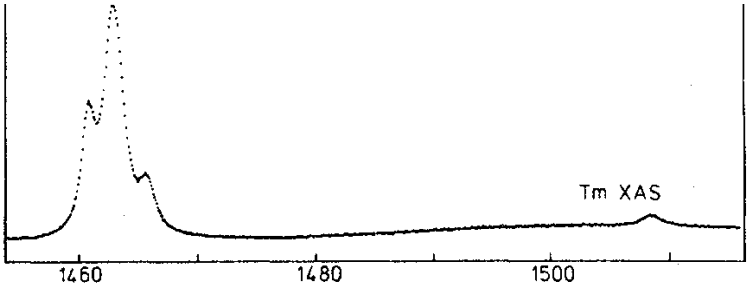
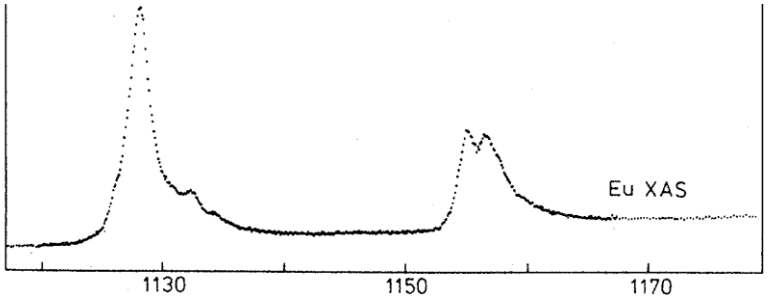
CTM4XAS: Tutorial exercises

Exercise 6: atomic multiplet spectra of rare earths



a) Calculate the 3d XAS spectrum of Tm metal. Try Tm2+, Tm3+ and Tm4+.
   Try also to switch off the valence band spin-orbit coupling.
b) What is the valence of Tm in Tm metal?
c) Why can one calculate the 3d XAS spectrum of Tm metal with an atomic calculation?



d) Calculate the 3d XAS spectrum of Eu metal. Try Eu2+, Eu3+ and Eu4+.
   Try also to switch off the valence band spin-orbit coupling.
e) What is the valence of Eu in Eu metal? Explain why.