CTM4XAS: Tutorial exercises

Exercise 3: manipulating the atomic multiplet spectrum of Ti3+

a) What is the configuration and ground state symmetry of Ti3+?
b) Calculate the atomic multiplet spectrum of Ti3+ (ti3b).
c) Set Fpd and Gpd to zero and repeat the calculation (ti3c).
d) Set Fpd, Gpd and the 2p spin-orbit coupling to zero (ti3d).
e) Set Fdd to zero and repeat the calculation (ti3e).
f) Set the 2p spin-orbit parameters to zero(ti3e).
g) Set the 3d spin-orbit coupling to zero(ti3g).