Rules for filling and removal of d-electrons

When filling orbitals:

a. The lowest energy orbitals will be filled first (e.g. 1s before 2s).
b. Orbitals of the same type (e.g. p) will only pair up electrons after there is one electron in each (e.g. you will get $2p_x^1\ 2p_y^1\ 2p_z^1$ rather than $2p_x^2\ 2p_y^1\ 2p_z^0$) – the Aufau principle.
c. The 4s orbital will always fill before the 3d orbital.
d. When forming ions, electrons will be removed from the 4s orbital before the 3d orbital.
e. For chromium and copper, an electron will be taken from the 4s orbital and placed in the 3d orbital to make half-full or full 3d orbitals respectively.

For filling the orbital order = 1s, 2s, 2p, 3s, 3p. 4s, 3d, 4p

Helpful hint - d-orbital occupation and electronic configurations

To be able to use Crystal Field Theory (CFT) successfully, it is essential that you can determine the **electronic configuration** of the central metal ion in any complex. This requires being able to recognize all the entities making up the complex and knowing whether the ligands are neutral or anionic, so that you can determine the **oxidation state** of the metal ion.

In many cases the oxidation state for first row transition metal ions will be either (II) or (III), but in any case you may find it easier to start with the M(II) from which you can easily add or subtract electrons to get the final electronic configuration.

A simple procedure exists for the M(II) case.

First write out all the first row transition metals with their symbols and atomic numbers:

22	23	24	25	26	27	28	29
Ti	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**

To see the number of electrons in the 3d orbitals then cross off the first 2, hence:

2	3	4	5	6	7	8	9

So, the electronic configuration of **Ni(II) is d^8** and the electronic configuration of **Mn(II) is d^5**.

What is the electronic configuration of Fe(III)?
Well, using the above scheme, Fe(II) would be d^6, by subtracting a further electron to make the ion more positive, the configuration of **Fe(III) will be d^5**.

Examples:
Cu = $4s^1$, $3d^{10}$, Cu^{2+} = $3d^9$
Cr = $4s^1$, $3d^5$, Cr^{3+} = $3d^3$

N.B. This simple procedure works fine for first row transition metal ions, but sorry it is no good for 2nd or 3rd row elements!