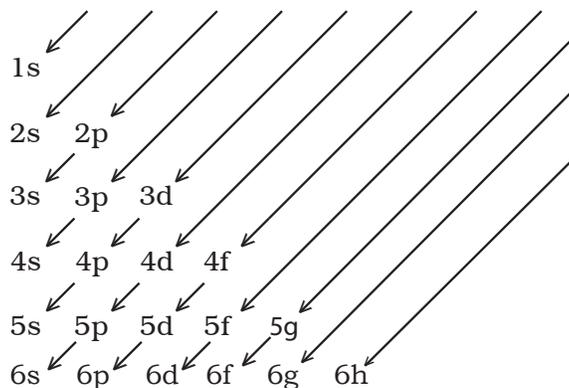


## Shells, Sub-shells and Orbitals, First Year Blog (for the week commencing the 27<sup>th</sup> of October 2019)

- a) • SHELLS are made up of sub-shells , and  
 • SUB-SHELLS are made up of orbitals, and  
 • an orbital is a volume of space in which an electron is most likely to be found, and one or two (but never more than two) electrons may occupy an ORBITAL.
- b) • Shell n=1 contains 1 sub-shell viz.<sup>1</sup> 1s  
 • Shell n=2 contains the 2 sub-shells viz. 2s 2p  
 • Shell n=3 contains the 3 sub-shells viz. 3s 3p 3d  
 • Shell n=4 contains the 4 sub-shells viz. 4s 4p 4d 4f  
 ..... and so on.
- c) • every 's' sub-shell contains only ONE orbital, and  
 • every 'p' sub-shell contains THREE orbitals, and  
 • every 'd' sub-shell contains FIVE orbitals, and  
 • every 'f' sub-shell contains SEVEN orbitals.  
*[NB Please note the progression 1, 3, 5, 7, ..... etc. You do not need to know about 'g' sub-shells for 'A' Level, but I am sure that you can work out how many orbitals they have!]*
- d) There is a specific order in which electrons go into orbitals, and the order in which the orbitals are filled is given by the grid below
- e) The orbitals in a SUB-SHELL are always filled singly until ALL the orbitals have one electron in them, and then only are the second electrons added in until the appropriate number of electrons has been achieved and it is very important that this rule **MUST** always be obeyed (other than for the exceptions of Chromium and Copper)!



- However, if you did electron configurations at GCSE Level, then you may have been taught something that will be very **unhelpful** to you at 'A' Level, so please now watch carefully and **UNLEARN** what you may have learnt at GCSE Level.

---

<sup>1</sup> The abbreviation "viz." stands for "namely" or "that is to say".

## REMOVING electrons rather than ADDING electrons

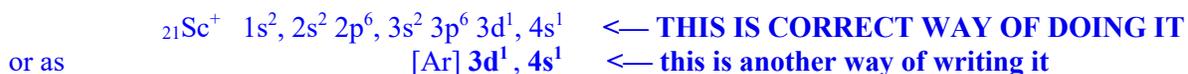
- In Chapter 1 and Chapter 2 we saw that a *positively* charged “ion” (i.e. a cation) is created by removing electrons from a neutrally charged species and that a *negatively* charged species (an anion) will be the result of adding/or forcing an electron onto a neutrally charged species – and now I want to look very briefly at the electron configuration of *ions*.
- On this page, I am not going to try to explain the rules for the removal of electrons, from an atom. All that I will do is to tell you how to do it.

- What I will confine myself to saying is this: if you look at the little grid on page 1 of this Chapter, you will see that the order of filling the orbitals 1s, 2s, 2p, 3s and 3p is very straightforward. It is only after 3p that you have to start being careful. After 3p you do NOT go on and start filling 3d – **instead you go to 4s and start filling that orbital!** Let us do the electron configuration of the first element where 3d starts to be filled i.e. the electron configuration for Scandium, Sc (cf. footnote<sup>2</sup>) viz



- Now, if you did electron configurations at GCSE Level, then could you please note very carefully that I did NOT write  ${}_{21}\text{Sc} \quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$  but instead I wrote  ${}_{21}\text{Sc} \quad 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^1, 4s^2$

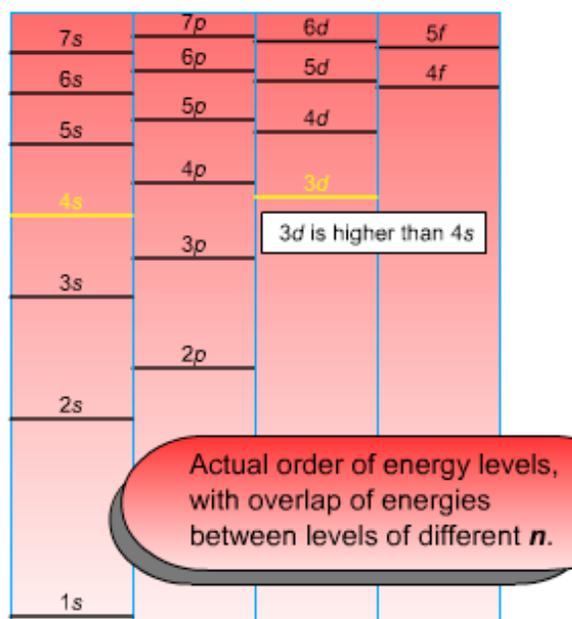
- There are two differences in the two configurations above viz. my configuration has commas at the end of each completed shell (*and this is a trivial thing that I do in order to differentiate one shell from another*), but the second difference is not trivial. I did NOT write the sub-shells in the order that I was putting the electrons into them. The reason for this is that when you come to do the electron configurations for **IONS**, then **you must remove electrons NOT in the order in which orbitals are filled, but instead you must remove them first of all from an orbital IN THE OUTERMOST SUB-SHELL CONTAINED IN THE OUTERMOST SHELL** – therefore if you use the GCSE notation, when you come to create the electron configuration for an ion you could get it wrong. As it happens, the *natural* ion of Scandium is  $\text{Sc}^{3+}$ , therefore you cannot get the electron configuration for the *natural* ion of Scandium wrong, but if you wanted to write the electron configuration for the first (*artificial*) ion of Scandium (i.e. the ion that would be created if you removed just *one* electron from an atom of Scandium), then if you used the GCSE notation for the atom and knocked off one electron, you would first have written  ${}_{21}\text{Sc} \quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$  and then **INCORRECTLY** have written  ${}_{21}\text{Sc}^+ \quad 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$  (← THIS IS WRONG) instead of correctly writing the  ${}_{21}\text{Sc}^+$  ion of Scandium as



- The ending for the artificial ion  ${}_{21}\text{Sc}^+$  is .....  **$3d^1, 4s^1$**  (and NOT .....  $3p^6 4s^2$ )!
- Let me therefore repeat my advice – do NOT write electron configurations according to the order in which orbitals are filled (even though you may have been taught to do so when you were learning GCSE Chemistry); but, instead, write your electron configurations in the SHELL order, **and then you will never get your electron configurations for IONS wrong.**

<sup>2</sup> You must familiarise yourself with the symbols for the names of all the different elements (or at very least for the first 36 elements in the Periodic Table – because that is what the ‘A’ Level syllabus requires you to know).

- I have said again and again that when you hear someone say something, you may think that you have understood what was said – but, in truth, you will not understand it until you have bashed the concepts around in your head and got to grips with them for yourself. Could I therefore urge you to practise writing out lots and lots of electron configurations for atoms and ions.
  - Let us have a look at the *electron configuration of ions* (and in fact we have already covered almost all that you need to know for this subject at ‘A’ Level).
- The factors that underlie electron configuration are (i) the physical distance of an electron from a nucleus (ii) the energy level that it occupies (iii) and the mutual repulsion between entities that possess a similar electrostatic charge.
  - The grid with the arrows on page 1 of this Chapter follows from the energy levels of the different sub-shells



Source : Professor Stephen Lower, Simon Fraser University

- The reason that (to create an ion) you remove electrons from ‘4s’ before ‘3d’ is because (with regard to distance) an **empty** ‘4s’ is farther away from the nucleus than ‘3d’, but an empty ‘4s’ has **LESS** energy than an empty ‘3d’. However, **when ‘3d’ starts having electrons put into it**, then (since electrons repel each other) the electrons in ‘3d’ are repelled by the electrons that have already been put in ‘4s’, and **the ones in ‘4s’ are now pushed farther away from the nucleus and go to a higher energy level than ‘3d’**. Once the ‘4s’ sub-shell starts to have electrons in it, **the ‘4s’ sub-shell is pushed physically up ABOVE the ‘3d’ sub-shell, and up above ‘3d’ in ENERGY terms also**.
- When creating an ion, the outermost electrons/the highest energy electrons must be removed FIRST, and THAT is why when you start taking electrons away to form an ion, the electrons in ‘4s’ MUST be removed before the electrons in ‘3d’**. They are both farther away from the nucleus than ‘3d’ electrons, AND they have more energy than ‘3d’ electrons.
- Isn’t it just lovely when you start to see how things work in Chemistry!