CHEM1611 Worksheet 2: Atomic Accountancy

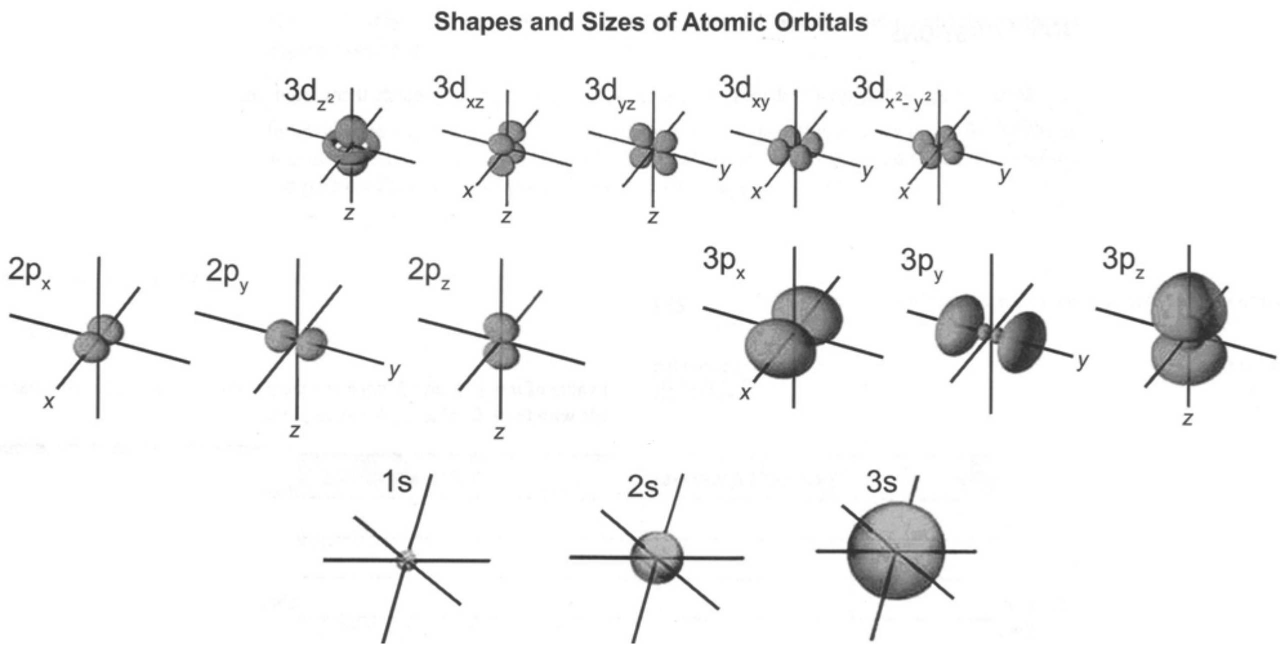
Model 1: Atomic Orbitals

Throughout history, the model of the atom and how/where the electrons exist and move has changed as our scientific knowledge has increased. The current model describes the motions of electrons using *atomic orbitals*. Orbitals gives us information about the *probability* of an electron being in a particular place around the nucleus. Orbitals have different shapes and sizes, depending on the energy of the electron.

To understand how orbitals work, we must first consider *quantum numbers*. Each electron has a set of four quantum numbers, each describing a certain property. There are four quantum numbers:

- n: the principal quantum number identifies the *size* and *energy* of the orbital. Its value can be any non-zero integer: 1, 2, 3, 4... with the size of the orbital increasing with n.
- l: the angular momentum quantum number identifies the *shape* of the orbital. For each value of n, it has values from 0 to (n-1). For historic reasons, a code is used for the l value:
  - l = 0 means an ***s* orbital**
  - l = 1 means a ***p* orbital**
  - l = 2 means a ***d* orbital**
  - l = 3 means an ***f* orbital**
- m_l: the magnetic orbital quantum number identifies the *subshell* and the orientation of the orbital For each value of l, it has values from l…0…-l
- m_s: the spin quantum number which describes the spin of the electron. It has values of +½ or -½ which are sometimes called 'spin up' and 'spin down' respectively. Each orbital can be used for a maximum of 2 electrons – one 'spin up' and one 'spin down'.

This all sounds very complicated! However, as you will see below, these quantum numbers lead to the Periodic Table and hence to all of chemistry (and so all biochemistry, biology, medicine etc.). The shapes and sizes of all of the orbitals with n = 1, 2 and 3 are shown below.



Critical thinking questions

1. What are the characteristic shapes of s, p, and d orbitals?

2. Which quantum number identifies the shape of an orbital?

3. For each value of n = 1, 2, and 3, what are the possible values for l, and what labels correspond to these orbitals? (*Hint*: re-read the *second* bullet point in Model 1.)

n	**Possible l values**	**Orbital labels**
1		
2		
3		

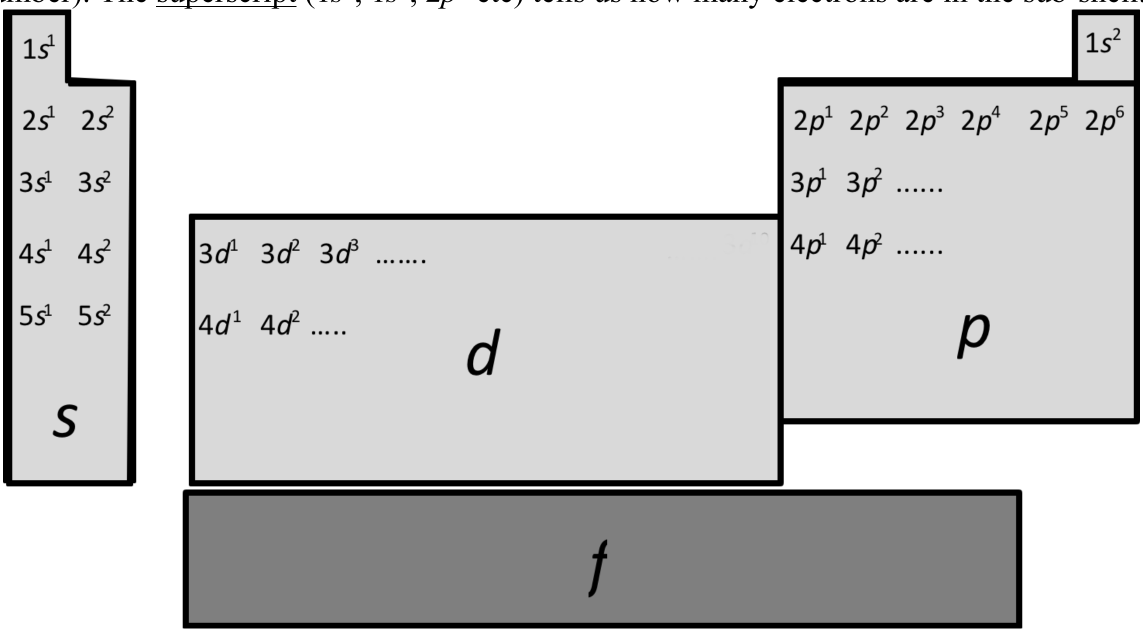
4. For each value of l = 0, 1, 2, what are the possible values for m_l? For each value of l, how many values can m_l have? (*Hint*: re-read the *third* bullet point in Model 1.). Complete the first 3 columns in the table below.

5. Complete the 4th column in the table below. (*Hint*: re-read the *fourth* bullet point in Model 1.)

l	**Possible m_l values**	**Number of values of m_l**	**Number of orbitals**	**Maximum number of electrons**
0				
1				
2				

Model 2: Electronic Configurations of Atoms

The *electronic configuration* of an atom provides information on which orbitals its electrons are in. The Periodic Table below shows how the orbitals are occupied by the valence electrons. The number in front of the orbital (1*s*, 2*s*, 2*p*, etc) gives the shell (the n quantum number). The *letter* (*s*, *p*, *d*, etc) gives the subshell (the l quantum number). The superscript ($1s^1$, $1s^2$, $2p^3$ etc) tells us how many electrons are in the sub-shell.



An element has the electronic configuration of the previous element plus an extra electron in the orbital shown on the figure. For example, H is $1s^1$ and He is $1s^2$. Li has the electron configuration of He plus one more electron so is $1s^2\ 2s^1$. The valence electrons of an atom are those in the outermost shell of the atom; core electrons are those in the completely filled inner shells.

Critical thinking questions

1. What are the electronic configurations the following elements?

(a) Li (b) Be (c) B (d) C

(e) N (f) O (g) F (h) Ne

2. What is the electronic configuration of the element that comes after Ne? What does it have in common with Li?

Box Notation

The table on the right shows the electron configurations of a series of atoms and introduces the *box representation* of atomic orbitals. The arrows indicate electrons, and the boxes indicate the orbitals. As there is a single *s* orbital in each shell, *s* orbitals are represented with a single box. As there are three *p* orbitals in each shell, *p* orbitals are represented by 3 boxes. The arrows show the spin ('up' or 'down') of the electrons.

- The ***Aufbau Principle*** says that electrons are added to the lowest energy atomic orbitals available.
- The ***Pauli Exclusion Principle*** says that no two electrons can have the same set of quantum numbers.
- ***Hund's Rule*** states that if multiple orbitals with the same energy are available, then electrons keep apart by occupying separate orbitals with spins pointing in the same direction if they can.

Atom	Electron configuration	Representation – only valence electrons!
H	$1s^1$	[↑]
He	$1s^2$	[↑↓]
Li	$1s^2 2s^1$ or [He] $2s^1$	[↑]
Be		[ ]
B	$1s^2 2s^2 2p^1$ or [He] $2s^2 2p^1$	[↑↓] [↑][ ][ ]
C	[He] $2s^2 2p^2$	[↑↓] [↑][↑][ ]
N		[ ] [ ][ ][ ]
O	[He] $2s^2 2p^4$	[↑↓] [↑↓][↑][↑]
Ne		[ ] [ ][ ][ ]
K	[Ar] $4s^1$	[ ]
Al		[ ] [ ][ ][ ]
Cl		[ ] [ ][ ][ ]

3. In reference to the *Aufbau principle*, what does the Periodic Table above tell you about the relative energies of the 2*s* and 2*p* orbitals?

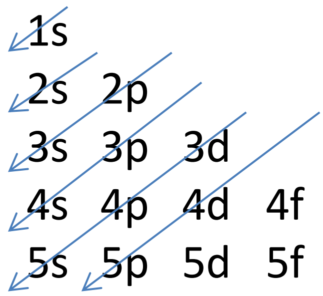
4. Which *Principle or Rule* do the up and down arrows in the table above refer to and which quantum number do they represent?

5. Which Principle or Rule explains the arrangement of the electrons in the *p* orbitals for C?

6. Fill in the missing electron configuration and box representations for Be, N, Ne, Al, Cl.

7. Why do you think we use the [X] substitution to shorten the electronic configuration (where [X] represents the electron configuration of the noble gas immediately before the element in question)? What is special about the electrons that are substituted in the place of [X]?

The figure on the right shows an easy way to remember the order in which atomic orbitals are filled. The arrows are followed starting from the top and remembering the ideas that you have discovered above:



- each *s* orbital can accommodate a maximum of 2 electrons
- each set of *p* orbitals can accommodate a maximum of 6 electrons
- each set of *d* orbitals can accommodate a maximum of 10 electrons
- each set of *f* electrons can accommodate a maximum of 14 electrons

8. What is the electron configuration of Fe? Give your answer using both long hand and the [X] shorthand.

9. What is the electron configuration of As?

Model 3: Electronic Configurations of Ions

The electronic configurations of cations and anions can be worked out from those of the neutral atoms by removing or adding electrons respectively:

- O has the electron configuration [He] $2s^2 2p^4$. O^{2-} has the electron configuration [He] $2s^2 2p^6$: the two electrons were added to the 2*p* orbitals.
- Mg has the electron configuration [Ne] $3s^2$. Mg^{2+} has the electron configuration [Ne] : the two electrons are removed from the 2*s* orbital.

Critical thinking questions

1. Draw the box representation for the valence electrons of O, O^{2-}, Mg and Mg^{2+}. What do you notice?

2. Write down the electronic configurations of the following ions.

   (a) S^{2-} (b) Al^{3+} (c) H^+ (d) H^-

Extension questions

1. Discuss within your group, the best position in the periodic table for H and He considering their chemical nature and their electronic configuration.

2. The first ionisation energy (I.E.) of the first 18 elements is plotted below. Identify the general trends that exist moving across a period and down a group of the periodic table and discuss in your groups the reasons why IE(B) < IE(Be) and IE(O) < IE(N).