# CHAPTER 1: Atomic Structure

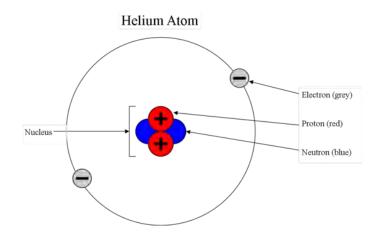
- 1.1 Inside the Atom
- 1.2 Isotopes

### Learning outcomes:

- (a) identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses.
- (b) deduce the behaviour of beams of protons, neutrons and electrons in electric fields.
- (c) describe the distribution of mass and charges within an atom.
- (d) deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge).
- (e) (i) describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number.
  - (ii) distinguish between isotopes on the basis of different numbers of neutrons present
  - (iii) recognise and use the symbolism  $\overset{\times}{y}A$  where x is the nucleon number and y is the proton number.

# 1.1 Inside the Atom

## Sub-atomic particles

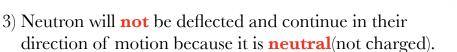


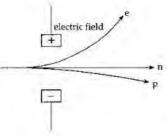
- 1) Electrons revolve around in region of space called orbitals.
- 2) Electrons **do not** move in fixed orbits.
- 3) The nucleus is made up of **protons and neutrons** which contains almost all the mass of the atom. This is because the mass of electrons is very small compared to others.
- 4) The nucleus is positively-charged because of the protons. Electrons, being negatively-charged, surround the nucleus.

Particles	Relative mass	Relative Charge	Charge / C
Protons, p	1	+1	+1.6 x 10 <sup>-19</sup>
Neutron, n	1	0	0
Electron, e	<u>1</u> 1836	-1	-1.6 x 10 <sup>-19</sup>

## Behaviour of sub-atomic particles in electric field

- 1) Proton will be deflected towards the **negative plate** because it is **positively-charged**.
- 2) Electron will be deflected towards the **positive plate** because it is **negatively-charged**.

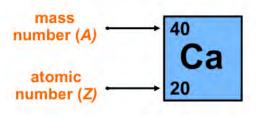




- 4) **Angle of deflection of electron > Angle of deflection of proton** because the mass of electron is smaller than proton. (angle of deflection is inversely proportional to charge/mass ratio)
- 5) Conclusion:
  - i. Protons are positively-charged
  - ii. Electrons are negatively-charged
  - iii. Neutrons are neutral
  - iv. Protons are much heavier than electron

### Nucleon number and proton number

- 1) Proton number is the total number of protons in an atom.
- 2) Nucleon number is the total number of protons and neutrons in an atom.
- 3) Proton number is also known as atomic number while nucleon number is also known as mass number.
- 4) In a neutral atom, the total number of protons **equals** to the total number of electrons.



- 5) When an atom gains or loses electrons, a cation or anion will be formed.
- 6) *Cation* is a positively-charged ion. It is formed when an atom **loses** electron(s). In cation, the number of protons is more than the number of electrons.
- 7) *Anion* is a negatively-charged ion. It is formed when an atom **gains** electron(s). In anion, the number of electrons is more than the number of protons.
- 8) An atom or ion is said to be
  - i. **isoelectronic** if they have the same number of electrons.
  - ii. **isotonic** if they have the same number of neutrons.
  - iii. **isotopic** if they have the same number of protons.

### To deduce the number of protons, neutrons and electrons in an atom/ion

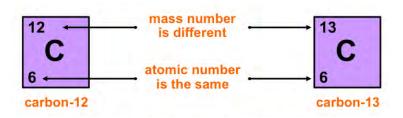
Atom/Ion	no. of protons	no. of neutrons	no. of electrons
<sup>16</sup> 80	8	16-8=8	8 + 0 = 8
17 O	8	17 - 8 = 9	8 + 0 = 8
<sup>18</sup> / <sub>8</sub> O	8	18 - 8 = 10	8 + 0 = 8
16 O 2-	8	16 - 8 - 8	8 + 2 - 10
35 17 Cl	17	35 - 17 = 18	17 + 0 = 17
37 17 C <i>l</i>	17	37 - 17 - 20	17 + 0 - 17
35 17 Cl -	17	35 - 17 = 18	17 + 1 = 18
14 N	7	14 - 7 = 7	7 + 0 = 7
<sup>14</sup> <sub>7</sub> N <sup>3-</sup>	7	14 - 7 = 7	7 + 3 = 10
73Li *	3	7 – 3 = 4	3 - 1 = 2
<sup>23</sup> <sub>11</sub> Na <sup>+</sup>	11	23 - 11 - 12	11 - 1 - 10
27 Al 3+	13	27 - 13 = 14	13-3=10
63 29 Cu +	29	63 - 29 = 34	29-1=28

# 1.2 Isotopes

## **Isotopes**

1) *Isotopes* are atoms of the same element with the same number of proton but different number of neutron.

Example:

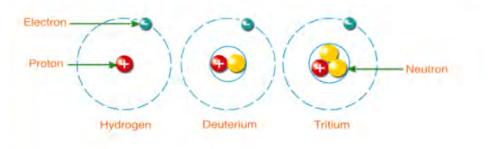


- 2) Isotopes have the **same**:
  - i. number of protons and electrons
  - ii. electronic configuration
  - iii. chemical properties(because they have the same number of electrons)

## 3) Isotopes have **different**:

- i. number of neutrons and nucleon number
- ii. mass
- iii. density
- iv. molecular speed
- 4) Isotopes can be stable or unstable. Unstable isotopes are called radioactive isotopes(radioisotopes).

Isotopic symbol	$^{1}_{1}$ H	2 H	3 H 1
Name	Protium	Deuterium	Tritium
Proton	1	1	1
Neutron	0	1	2
Electron	1	1	1



# CHAPTER 2: Atoms, Molecules and Stoichiometry

- 2.1 Mass of Atoms and Molecules
- 2.2 Mass Spectrometer
- 2.3 Amount of Substance
- 2.4 Empirical Formula and Molecular Formula
- 2.5 Stoichiometry and Equations

#### Learning outcomes:

- (a) define and use the terms relative atomic, isotopic, molecular and formula masses, based on the C-12 scale.
- (b) define and use the term mole in terms of the Avogadro constant.
- (c) analyse mass spectra in terms of isotopic abundances [knowledge of the working of the mass spectrometer is not required].
- (d) calculate the relative atomic mass of an element given the relative abundances of its isotopes, or its mass spectrum.
- (e) define and use the terms empirical and molecular formulae.
- (f) calculate empirical and molecular formulae, using combustion data or composition by mass.
- (g) write and/or construct balanced equations.
- (h) perform calculations, including use of the mole concept, involving:
  - (i) reacting masses (from formulae and equations).
  - (ii) volumes of gases (e.g. in the burning of hydrocarbons).
  - (iii) volumes and concentrations of solutions.

When performing calculations, candidates' answers should reflect the number of significant figures given or asked for in the question. When rounding up or down, candidates should ensure that significant figures are neither lost unnecessarily nor used beyond what is justified.

(i) deduce stoichiometric relationships from calculations such as those in (h).

# 2.1 Mass of Atoms and Molecules

# Concept of relative mass

- 1) Relative mass is an indication of how heavy is an atom compared to another atom which is used as a standard model.
- 2) Relative mass is expressed in atomic mass unit(a.m.u).
- 3) C-12 was chosen to be the standard model because:i. it is the most abundant isotope of carbonii. it is a solid, easy to handle and easily available
- 4) C-12 was assigned a mass of exactly 12 a.m.u.. This is known as C-12 scale.
- 5) For example, an atom which is 3.5 times heavier than a C-12 atom would have a relative mass of  $(3.5 \times 12) = 42$  a.m.u.. That means, this atom is 42 times heavier than the mass of  $(1/12 \times 12) = 12$  atom).

# Relative isotopic mass

1) *Relative isotopic mass* is the mass of an isotope measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

## Relative atomic mass, Ar

1) *Relative atomic mass, Ar* is the weighted average relative masses of all its isotopes measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.

Relative atomic mass, Ar =	Average mass of one atom of the element	X 12
	Mass of one atom of carbon-12	

Example:

Ratio of Cl-35 to Cl-37 is 3:1. If you have 4 typical atoms of chlorine, total mass is  $(35 \times 3) + (37 \times 1) = 142$ . So, the average mass of the isotopes is 142/4 = 35.5.

This implies that 35.5 is the **relative atomic mass** of chlorine while 35 is the **relative mass** of Cl-35 and 37 is the **relative mass** of Cl-37.

### Relative molecular mass, Mr

- 1) *Relative molecular mass, Mr* is the weighted average of the masses of the molecules measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.
- 2) It should only be applied to substances which exist as molecules.
- 3) It is found by adding up all the relative atomic masses of all the atoms present in the molecule.
- 4) Examples:
  i. Mr (H<sub>2</sub>O) = 2(1) + 16 = 18
  ii. Mr (CHCl<sub>3</sub>) = 12 + 1 + 3(35.5) = 119.5

### Relative formula mass, Mr

- 1) *Relative formula mass, Mr* is the weighted average of the masses of the formula units measured on a scale in which a carbon-12 atom has a mass of exactly 12 units.
- 2) It works for both ionic and covalent compounds.
- 3) Examples:
  - i. Mr (NaCl) = 23 + 35.5 = 58.5
  - ii. Mr (CuSO<sub>4</sub> · H<sub>2</sub>O) = 64 + 32 + 4(16) + 5[2(1) + 16] = 249.5

# 2.2 Mass Spectrometer

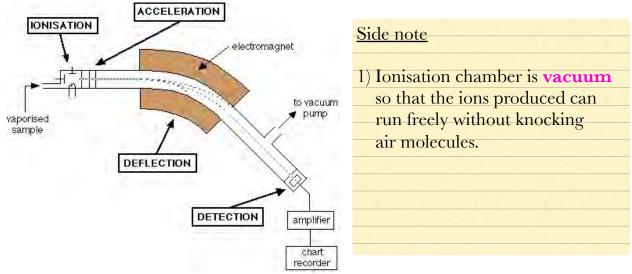
### What is mass spectrometer?

- 1) A mass spectrometer is used to determine:
  - a. relative isotopic mass
  - b. relative abundance of isotopes
  - c. relative atomic mass
  - d. relative molecular mass
  - e. structural formula of compounds

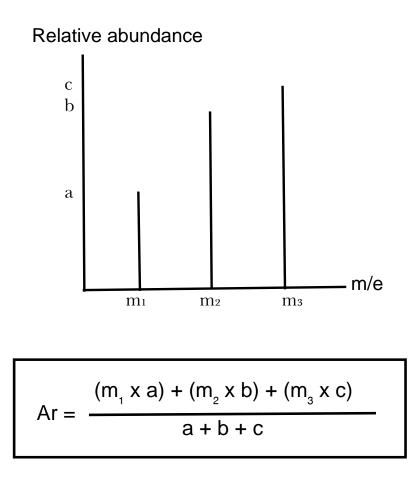
### Determination of relative atomic mass using mass spectrometer

1) Five steps:

- i. Vaporisation
  - atoms are vaporised to form **gaseous atom**.
- ii. Ionisation
  - gaseous atoms are bombarded with high energy electrons to form positive ions.
- iii. Acceleration
  - the ions are accelerated so that they have the same kinetic energy.
- iv. Deflection
  - ions are deflected by a magnetic field. The amount of deflection depends on:
    - 1) the mass of the ion
    - 2) the amount of positive charge on it
  - the larger the mass, the smaller the deflection.
  - the higher the charge, the larger the deflection.
  - the two factors combine into mass/charge ratio (m/e or m/z).
  - the smaller the value of m/e, the larger the deflection
- v. Detection
  - the beam of ions are detected electrically.
  - the data are fed into the computer and the mass spectrum is produced.

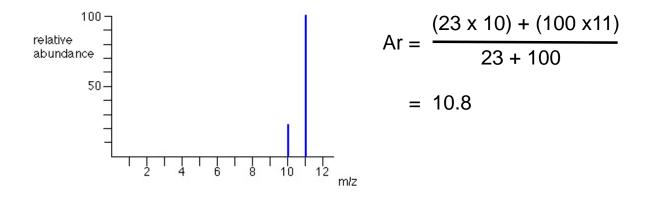


Mass spectrum (How to calculate relative atomic mass, Ar from it?)



Example:

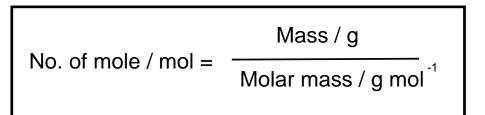
The mass spectrum of boron, **B** is as shown, given the relative abundances: B-10:23B-11:100



# 2.3 Amount of Substance

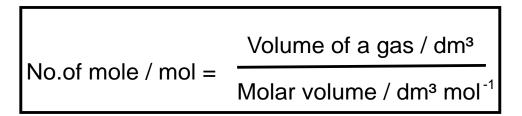
The mole and the Avogadro's constant

- 1) A *mole* of a substance is the amount of substance that contains the same amount of stated elementary units as there are atoms in 12 g of C-12.
- 2) The number of atoms is 12 g of C-12 is 6.02 x 10<sup>23</sup>. This number is also known as the **Avogadro's constant**, *L*.
- 3) Examples:
  - i. 1 mol of He contains  $6.02 \times 10^{23}$  He **atoms**.
  - ii. 1 mol of CO<sub>2</sub> contains  $6.02 \times 10^{23}$  CO<sub>2</sub> molecules but  $3 \times (6.02 \times 10^{23})$  atoms.
- iii. 1 mol of NaCl contains 6.02 x 10<sup>23</sup> NaCl units, Na<sup>+</sup> and Cl<sup>-</sup> ions.



## Moles and volumes

- 1) Volume occupied by a gas depends on the amount of gas, temperature and pressure. In other words the volume of a gas is not fixed.
- 2) *Avogadro's law* states that for equal volumes of all gases, under the same conditions, contain the same number of moles.
- 3) Hence, equal number of moles of any gas, under the same conditions, would occupy the same volume. It does not depend on the nature of gas.
- 4) At room temperature of 20  $^{\circ}\!\mathrm{C}$  and a pressure of 1 atm, one mole of any gas occupies 24 dm<sup>3</sup>.
- 5) At standard temperature and pressure (s.t.p), which is 0 °C and 1 atm, one mole of any gas occupies 22.4 dm<sup>3</sup>.



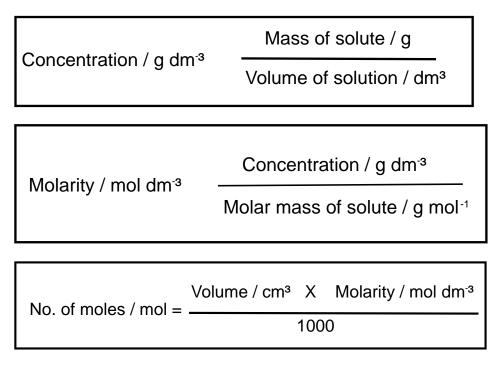
6) i. Complete combustion of hydrocarbon produces water and carbon dioxide. The general equation is as follow:

$$C_x H_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow x CO_2 + \left(\frac{y}{2}\right) H_2 O$$

ii. In incomplete combustion, the possible products are carbon dioxide, carbon monoxide, carbon soot and water.

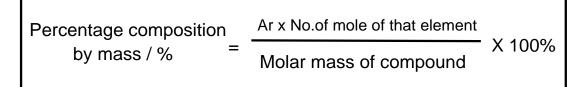
Moles and concentration of solutions

- 1) A solution is a homogeneous mixture of two or more substance.
- 2) The substance presents in small quantity is called the solute while the substance present is larger quantity is called the solvent.
- 3) Concentration is the amount of solute present in a fixed quantity of solution.
- 4) Concentration is expressed in terms of g dm<sup>-3</sup>. Concentration in mol dm<sup>-3</sup> is called molar concentration or **molarity**.



# 2.4 Empirical Formula and Molecular Formula

Percentage composition by mass



## Empirical formula

- 1) *Empirical formula* is a chemical formula that shows the simplest ratio of the atoms that combine to form a molecule.
- 2) Steps to find empirical formula:
  - i. Find the mass of each element.
  - ii. Find the number of mole of each element (divide by its Ar).
  - iii. Find the simplest ratio (divide by the smallest number).
  - iv. Construct the empirical formula using the simplest ratio.

[ If a decimal or fraction exists, round up or eliminate the fraction ] [ Never assume a formula ]

# 3) Some facts:

- i. The formula for an ionic compound is always its empirical formula.
- ii. The empirical formula and molecular formula for simple inorganic molecules are often the same.
- iii. Organic molecules have different empirical and molecular formula.

# Molecular formula

- 1) *Molecular formula* is a chemical formula that shows the actual number of atoms that combine to form the compound.
- 2) In order to deduce the molecular formula of a compound, we need to know:i. the relative formula mass of the compound.
  - ii. the empirical formula of the compound.

# Principle of conservation of mass

- 1) Mass is neither created nor destroyed during a chemical reaction. Therefore the total mass of the reactants is equal to the total of the products in a closed system.
- 2) For example, the total mass of iodine in the reactants is equal to the total mass of iodine in the products.
- 3) This can be used to solve problems in calculating the empirical formula.

# 2.5 Stoichiometry and Equations

# Stoichiometry

- 1) Stoichiometry is the proportion of things either reacting or combining.
- 2) In compounds, it refers to the ratio in which the atoms are combined together. For example, water, H<sub>2</sub>O has a stoichiometry of 2 hydrogen to 1 oxygen.
- 3) It also refers to the reacting proportions in a chemical equation. For example:  $2H_2 + O_2 \rightarrow 2H_2O$

The stoichiometry shows that 2 moles of hydrogen react with 1 mole of oxygen to form 2 moles of water.

### Ionic equations

- 1) Steps to construct net ionic equations:
  - i. Write the balanced molecular equation.
  - ii. Write the complete ionic equation by splitting it into ions(if possible).
- iii. Cancel out the spectator ions. (Spectator ions are ions that present in the mixture but do not participate in the reaction.)
- iv. Write down the 'leftovers', that is the net ionic equation.

Chemical equation:  $HCl_{(aq)} + NaOH_{(aq)} \rightarrow NaCl_{(aq)} + H_2O_{(I)}$ 

Complete ionic equation:  $H^+CF_{(aq)} + Na^+OH^-_{(aq)} \rightarrow Na^+CF_{(aq)} + H_2O_{(I)}$ 

Net ionic equation:  $H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(I)}$ 

# FAQ 1: When to split compounds into ions?

1) Only split aqueous ionic compounds. For example, NaCl(aq) and HCl(aq)

 Do not split solid ionic compounds and covalent compounds, as well as metals.
 For example, NaCl(s), H2O(l), Mg(s) and HCl(g)

### FAQ 2: How to identify spectator ions?

1) The ions present on both sides of the equation are spectator ions.

# CHAPTER 3: Electrons in Atoms

- 3.1 Sub-shells and Atomic Orbitals
- 3.2 Electronic Configuration
- 3.3 Ionisation Energy

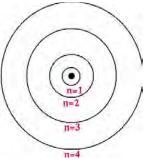
### Learning outcomes:

- (a) describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals.
- (b) describe the shapes of s and p orbitals.
- (c) state the electronic configuration of atoms and ions given the proton number (and charge), using the convention 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup> etc.
- (d) (i) explain and use the term ionisation energy.
  - (ii) explain the factors influencing the ionisation energies of elements.
  - (iii) explain the trends in ionisation energies across a Period and down a Group of the Periodic Table.
- (e) deduce the electronic configurations of elements from successive ionisation energy data.
- (f) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table.

# 3.1 Sub-shells and Atomic Orbitals

# Principle quantum shell

- 1) Electrons are arranged outside the nucleus in **energy levels** or **principle quantum shell, n**.
- 2) The principal quantum shells are numbered according how far are they from the nucleus.
- 3) The lowest energy level, n = 1 is closest to the nucleus, the energy level n = 2 is further out, and so on.
- 4) The electrons in energy level further away from the nucleus have more energy and held less tightly by the nucleus.
- 5) Electrons **do not** move in fixed circular paths, they occupy a space called the atomic orbitals.



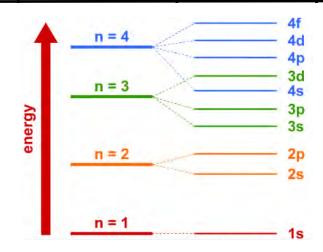
The circles represent energy levels

6) The total number of electrons that can occupy any principal shell is 2n<sup>2</sup>, where n is the principal quantum number.

## Quantum sub-shells

- 1) The principal quantum shells, apart from the first, are split into sub-shells. Each principle quantum shell contains a different number of sub-shells.
- 2) The first energy level contains one sub-shell, the second energy level contains two and so on.
- 3) The sub-shells are distinguished by letters s, p, d, f and so on.
- 4) The energy of electrons in the sub-shells increases in the order s .

Principal quantum shell	Maximum number of electrons	Number of sub-shells	Name of sub-shells
K, n = 1	2	1	1s
L, n = 2	8	2	2s, 2p
M, n = 3	18	3	3s, 3p, 3d
N, n = 4	32	4	4s, 4p, 4d, 4f



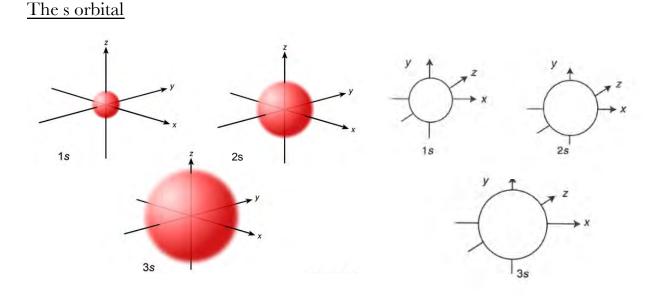
## The impossibility of drawing orbits for electrons

- 1) Heisenberg Uncertainty Principle says, you cannot know with certainty where an electron is and where it is going next.
- 2) This makes it impossible to draw out an orbit or pathway in which the electrons move.

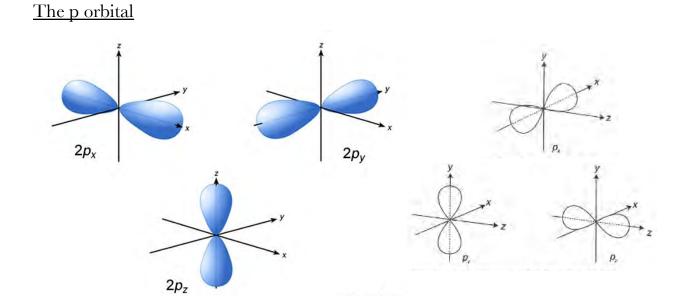
## Atomic orbitals

- 1) An *atomic orbital* is a region of space around the nucleus where the probability of finding a particular electron is maximum (>95%).
- 2) The sub-shells are split further into orbitals where the electrons are placed.

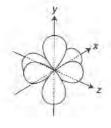
- 3) The number of orbital in each sub-shell depends on the sub-shells.
   s one orbital {s}
   p three orbitals {px, py, pz}
  - d five orbitals { $d_{xy}$ ,  $d_{yz}$ ,  $d_{xz}$ ,  $d_{x^2-y^2}$ ,  $d_{z^2}$ }
- 4) Orbitals having the same energy are called degenerate orbitals. For example,  $p_x$ ,  $p_y$  and  $p_z$  are degenerate orbitals.
- 5) The concept of orbitals arises from the fact that an electron has dual nature. It behaves as a particle as well as a wave.
- 6) In the **nth** principal quantum shell, there are **n** sub-shells, **n**<sup>2</sup> orbitals and a maximum of **2n**<sup>2</sup> electrons.



- 1) All the s orbitals are **spherical** and **non-directional**.
- 2) The shaded region represents the region in which the chance of finding the s electron is more than 95%.
- 3) The size of the s orbital increases in the order 1s < 2s < 3s < 4s.



- 1) All the p orbitals are **dumb-bell shaped** and **directional**.
- 2) p orbitals are only available from the second principal quantum shell and onwards.



- 3) There are 3 types of p orbitals,  $p_x$ ,  $p_y$  and  $p_z$ . All 3 different types of p orbitals are perpendicular to each other along the x, y and z axes.
- 4) Going to a higher energy level, the 'lobes' of the p orbital become longer.

