# ATOMIC STRUCTURE

**Content:**

- The nucleus of the atom: neutrons and protons, isotopes, proton and nucleon numbers
- Electrons: electronic energy levels, ionisation energies, atomic orbitals, extranuclear structure (empty space around the nucleus where electrons can be found)

**Learning Outcomes required for H1 (8873) & H2 (9729) Chemistry:**

Students should be able to:

(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 an electric field
(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) describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number
(f) 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
(g) describe the shapes of s, p and d orbitals [knowledge of wave functions is not required]
(h) state the electronic configuration of atoms and ions given the proton number (and charge)
(i) explain the factors influencing the ionisation energies of elements
(j) deduce the electronic configurations of elements from successive ionisation energy data
(k) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table

## 1. INTRODUCTION

The interactions between the valence electrons of 2 or more atoms lead to chemical combinations between them. Hence the chemical properties of an element are largely determined by the number of valence electrons each of its atoms possesses.

The study of the electronic structure of atoms, i.e. the detailed arrangement of electrons of an atom, is therefore of fundamental importance in the understanding of chemical behaviors of elements.

**Success criteria:**

- Identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses.
- Define nucleon number (mass number) and proton number (atomic number).
- Deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge).

### 1.1 What are sub-atomic particles?

Atoms are made up of 3 types of particles (known as sub-atomic particles).

| Sub-atomic Particle | | Relative charge | Relative mass |
|---|---|---|---|
| proton (*p*) | Collectively known as '*nucleons*'. | +1 | 1 |
| neutron (*n*) | | 0 | 1 |
| electron ($e^-$) | | –1 | 1/1840 |

**Note:**
As the mass of electron is insignificant compared to mass of *p* & *n*.
*Nucleon number = mass number*

**Note:**
Atoms are **electrically neutral**
(no. of *p* = no. of $e^-$)

Loss of $e^-$ gives rise to cation
(no. of *p* > no of $e^-$)

Gain of $e^-$ gives rise to anion
(no. of $e^-$ > no of *p*)

### 1.2 Proton Number and nucleon Number

Nucleon number (mass number)

- total number of protons and neutrons in an atom

Proton number (atomic number)

- number of protons in an atom
- determines the chemical identity of an atom.
- indicates the number of electrons in an electrically *neutral* atom

$^{35}_{17}Cl$

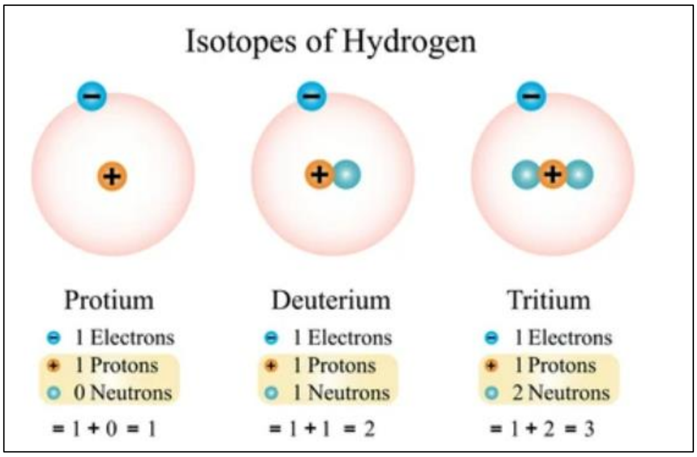
Chlorine-35

**Success criteria:**
- Recognise that only the proton number determines the chemical identity of an atom.

## 1.3 Isotopes

Atoms of the same element do not all have the same mass. **Isotopes** are **atoms of the same element that have the same proton number but different nucleon number (different number of neutrons).**

Isotopes of an element have the same electronic configuration and chemical properties. They have different relative isotopic masses and physical properties.




**Note:**
*When referring to a particular isotope, the nucleon number and the proton number must be indicated.*
e.g. if we want to refer to deuterium, we should write ${}^{2}_{1}H$ for clarity.

**<u>Checkpoint 1</u>** 

**1** State the number of protons, electrons and neutrons for the following particles:

| Particles | Nucleon number | No. of protons | No. of neutrons | No. of electrons |
|---|---|---|---|---|
| ${}^{31}_{15}P$ | | | | |
| ${}^{40}_{20}Ca^{2+}$ | | | | |
| ${}^{32}_{16}S^{2-}$ | | | | |

Generally, **except for ${}^{1}_{1}H$, number of neutrons ≥ number of protons** for other elements.

**2** Which of the ions has more electrons than protons and more protons than neutrons?
[Given: ${}^{4}_{2}He$, ${}^{1}_{1}H$, ${}^{16}_{8}O$, $D = {}^{2}_{1}H$]

**A** $He^{+}$ **B** $OH^{-}$ **C** $D_3O^{+}$ **D** $OD^{-}$

**3** Oxygen has two isotopes, $^{16}O$ and $^{18}O$. An oxide ion, $^{x}_{8}O^{y-}$ has the same number of neutrons and electrons.

What could be the values of *x* and *y*?

| | *x* | *y* |
|---|---|---|
| **A** | 16 | 1 |
| **B** | 16 | 2 |
| **C** | 18 | 1 |
| **D** | 18 | 2 |

**4** In 1999 Russian chemists claimed to be the first to identify atoms of a new element of proton number 114. This was produced by bombarding atoms of plutonium, Pu, with the atoms of an isotope of a group 2 element, **X**. The reaction taking place is as shown below.

$$^{244}_{94}Pu + \boldsymbol{X} \rightarrow \mathbf{^{289}_{114}}[new\ element] + 3\ neutrons\ (^{1}_{0}n)$$

What is **X**?

**A** Mg **B** Ca **C** Sr **D** Ba

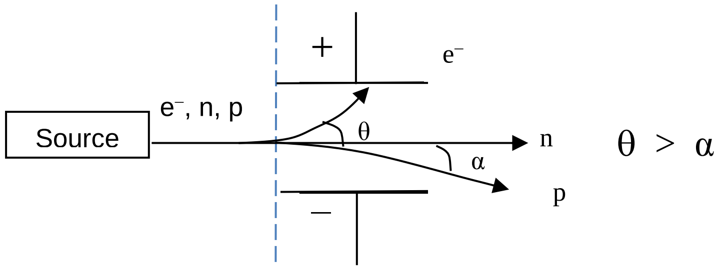
***[N03/1/4]***

**Success criteria:**
- Able to deduce the direction of subatomic particles (protons, neutrons and electrons) and charged particles in an electric field.
- Able to compare the angle of deflection by considering their $\frac{charge}{mass}$ ratio.

### 1.4 Effect of an electric field on protons, neutrons and electrons

Protons and electrons, being charged particles, are deflected by an electric field.

The angle of deflection, θ, is proportional to the $\frac{\text{charge}}{\text{mass}}$ ratio of the particles.



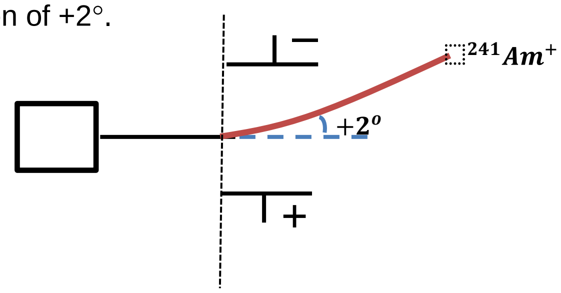

**Note:**
*e*⁻ is deflected to a greater extent than *p* because of its much smaller mass.

Angle of deflection in an electric field depends on:
- charge of particle: The greater the charge, the greater the extent of deflection.
- mass of particle: The greater the mass, the smaller the extent of deflection.

$$\boxed{\textbf{angle of deflection} \propto \frac{\textbf{charge}}{\textbf{mass}}}$$

***Worked Example 1***

A sample of the element Americium (Am) was vaporised, ionised and passed through an electric field. It was observed that a beam of $^{241}Am^{+}$ particles gave an angle of deflection of +2°.




**Note:**
Ions are attracted to the oppositely charged plate and the angle has to be indicated as + or – relative to the reference line.

Assuming an identical set of experimental conditions, by what angle would a beam of $^{32}S^{-}$ particles be deflected?

$$\theta = k \times \frac{\text{charge}}{\text{mass}}$$

For $^{241}Am^{+}$,

$+2 = k \times \frac{+1}{241}$

k = 482

For $^{32}S^{-}$,

angle of deflection of $^{32}S^{-}$ $= 481 \times \frac{-1}{32}$

$= -15.1°$

**Success criteria:**
- Able to define terms relative atomic mass and relative isotopic mass.
- Able to calculate the relative atomic mass of an element given the relative abundances of each isotope.

## 2 Quantifying the masses of atoms

In section 1, we have looked at the composition of the atom. While the protons, neutrons and electrons have masses, they are so small that it is impossible to weigh the atoms individually. Thus for everyday use, we usually measure the *relative* masses of atoms, or how heavy one atom is compared to another atom.

### 2.1 Relative Masses of atoms

All relative atomic mass are measured against the most abundant isotope of carbon.

$$Relative\ atomic\ mass, A_r = \frac{weighted\ average\ mass\ of\ one\ atom\ of\ an\ element}{\frac{1}{12} \times the\ mass\ of\ one\ atom\ of\ ^{12}C}$$

**Note**: ‘Weighted average’ is used because in the calculation of $A_r$, the relative abundances of all possible isotopes of that element are taken into account.
In cases where we want to deal specifically with the atomic mass of a particular isotope, the term *relative isotopic mass* is used.

$$Relative\ isotopic\ mass = \frac{mass\ of\ one\ atom\ of\ an\ isotope\ of\ an\ element}{\frac{1}{12} \times the\ mass\ of\ one\ atom\ of\ ^{12}C}$$

### 2.2 Relative abundance of isotopes

Most elements consist of mixtures of isotopes. The abundance of each isotope in a mixture is called the **isotopic abundance** or the **relative abundance.**

The relative atomic mass of an element is also the sum of the relative isotopic masses of each isotope multiplied by their relative abundances.

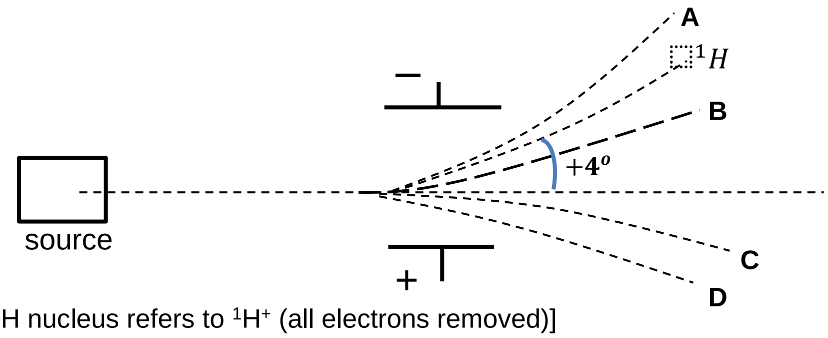
## Checkpoint 2

**1** *Use of the Data Booklet is relevant to this question.*

Which of the ions will be deflected the **most** in an electric field?

**A** $S^{2-}$ **B** $Br^{-}$ **C** $F^{-}$ **D** $O^{2-}$

**2** When passed through an electric field, the $^{1}H$ nucleus is deflected as shown below.




[**Note:** $^{1}H$ nucleus refers to $^{1}H^{+}$ (all electrons removed)]

Which of the above beams represents the deflection for an ion $^{2}X^{2-}$?

**3** A plasma is a gaseous mixture in which atoms have been completely stripped of their electrons, leaving bare nuclei. When passed through an electric field, the $^{1}H$ nucleus is deflected at an angle of +4°. What will be the angle of deflection for the $^{3}H$ nucleus in the same plasma?

**A** +0.75° **B** +1.3° **C** +4° **D** +12°

**4** The five isotopes of krypton occur in the following abundances:

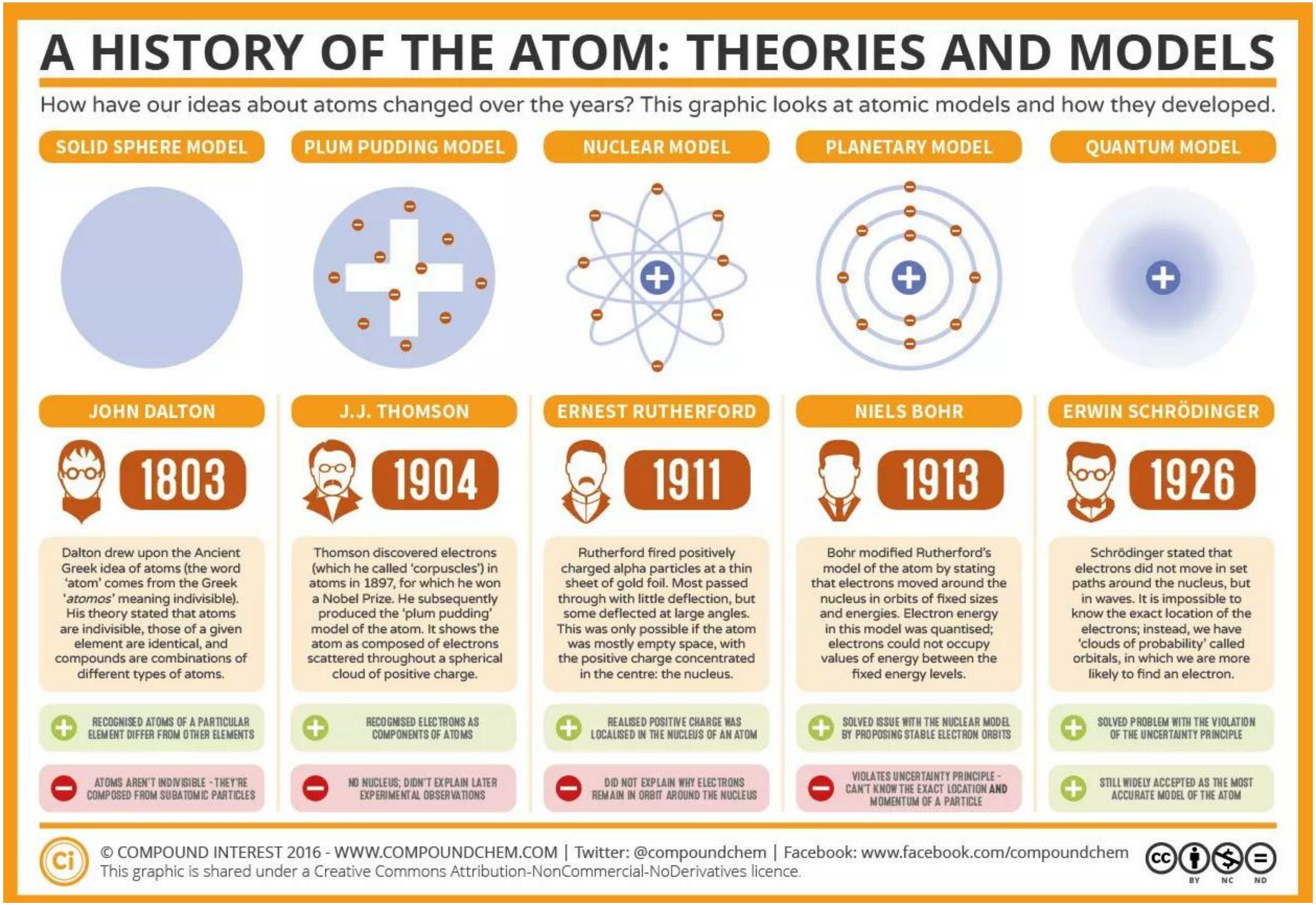
| Isotopic mass | % abundance |
|---|---|
| 80 | 2 |
| 82 | 12 |
| 83 | 12 |
| 84 | 57 |
| 86 | 17 |

Use these data to calculate a value, to one decimal place, for the $A_r$ of the atmospheric krypton.

**5** The relative atomic mass of boron, which consists of the isotopes $^{10}_{5}B$ and $^{11}_{5}B$ is 10.8.

What is the percentage of $^{11}_{5}B$ atoms in the isotopic mixture?

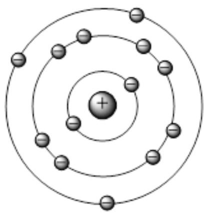
## 3 HISTORY OF THE ATOMIC MODEL



## 3. HISTORY OF THE ATOMIC MODEL

The atomic model has evolved over time with the surfacing of new evidence relating to the structure of an atom. Through this development of the atomic model, you will be able to relate the various understandings of the atomic structure to the different atomic models proposed in history. For e.g. the idea of an atom as in indivisible particle is based on the particle model; the idea of the presence of subatomic particles and electrons orbiting the nucleus is based on the nuclear model; the idea of electrons in multiple orbits and electrons in discrete energy levels is based on Bohr's model; and the idea of electrons in terms of probable space and different shapes of orbitals is based on the quantum model.

**What you have learnt:**



Based on Bohr, electronic configuration of A*l* will be 2.8.3

According to Bohr, electrons move around the nucleus in **fixed orbits** or **shells**. The electrons in each shell have different energy levels. The shells closed to the nucleus have lower energy levels than those further away.

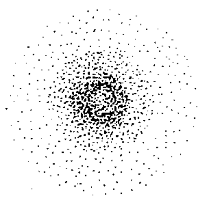
Each shell can hold a maximum number of electrons. The first shell can hold a maximum of 2 electrons, the second shell 8 and the third shell 18 and so on. The electrons are filled from the lowest energy level before going to the next level.

However, the Bohr's model is **not an accurate representation** as the electrons are **not orbiting** round the nucleus.

Electrons move around the nucleus in electronic shells of fixed energy levels described by numbers known as the **principal quantum numbers (*n*).**

The larger the *n* ➔ the greater the energy level of the principal quantum,
➔ the further the electronic shell is from the nucleus.

Each energy level (principal quantum shell) is made up of subshells (known as s, p, d, f subshells), which are in turn made up of orbitals.



**H atom**
Every dot represents a location where the electron is most likely to be found.

An **orbital** is a **region of space** in which there is a high probability of finding an electron (although the electron is not confined to this region). The shape of the orbitals will depend on the energy of the electron. When an electron is in an orbital of higher energy it will have a higher probability of being found further from the nucleus.

Each orbital can accommodate **2 electrons.**

**Success criteria:**
- 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
- Able to draw the s, p and d orbitals on x, y and z axis, showing their shapes and orientation in space accurately.
- Able to describe the shapes of s and p orbitals and recognize that their size increases with n.

### 3.1 Principal Quantum Shells, Subshells and Orbitals

Atom *consists of* nucleus, Principal quantum shells

nucleus *is made up of* protons, neutrons

Principal quantum shells *are made up of* subshells

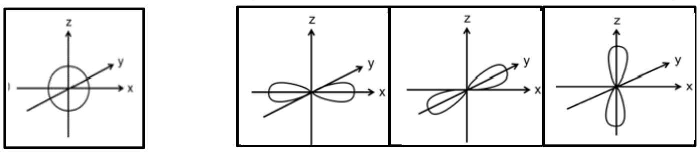
subshells *are made up of* orbitals

orbitals *containing* electrons

**Principal Quantum Shell**
(n = 1, 2, 3 …)

**s subshell**
(1 × s orbital)

**p subshell**
(3 × p orbitals)



s orbital
**spherical shape**

p orbital p orbital p orbital
**Dumb-bell shape**

[Each orbital can accommodate a maximum of 2 electrons]

**Note:**
Each orbital can accommodate a maximum of 2 electrons

| Principal Quantum No. | Types of subshell | No of orbitals | Types of orbitals | Total no. of orbitals ($n^2$) | Max. no of $e^-$ in the PQS ($2n^2$) |
|---|---|---|---|---|---|
| ***n*** = 1 | 1s | 1 | 1s | 1 | 2 |
| ***n*** = 2 | 2s | 1 | 2s | 4 | 8 |
| | 2p | 3 | $2p_x$, $2p_y$, $2p_z$ | | |
| ***n*** = 3 | 3s | 1 | 3s | 9 | 18 |
| | 3p | 3 | $3p_x$, $3p_y$, $3p_z$ | | |
| | 3d | 5 | $3d_{xy}$, $3d_{xz}$, $3d_{yz}$, $3d_{x^2-y^2}$, $3d_{z^2}$ | | |
| ***n*** = 4 | 4s | 1 | 4s | 16 | 32 |
| | 4p | 3 | $4p_x$, $4p_y$, $4p_z$ | | |
| | 4d | 5 | $4d_{xy}$, $4d_{xz}$, $4d_{yz}$, $4d_{x^2-y^2}$, $4d_{z^2}$ | | |
| | 4f | 7 | *Not in syllabus* | | |

### 3.2 Relative Energies of the Orbitals

Within each principal quantum shell, the energy of the electron depends on the subshell it is in.

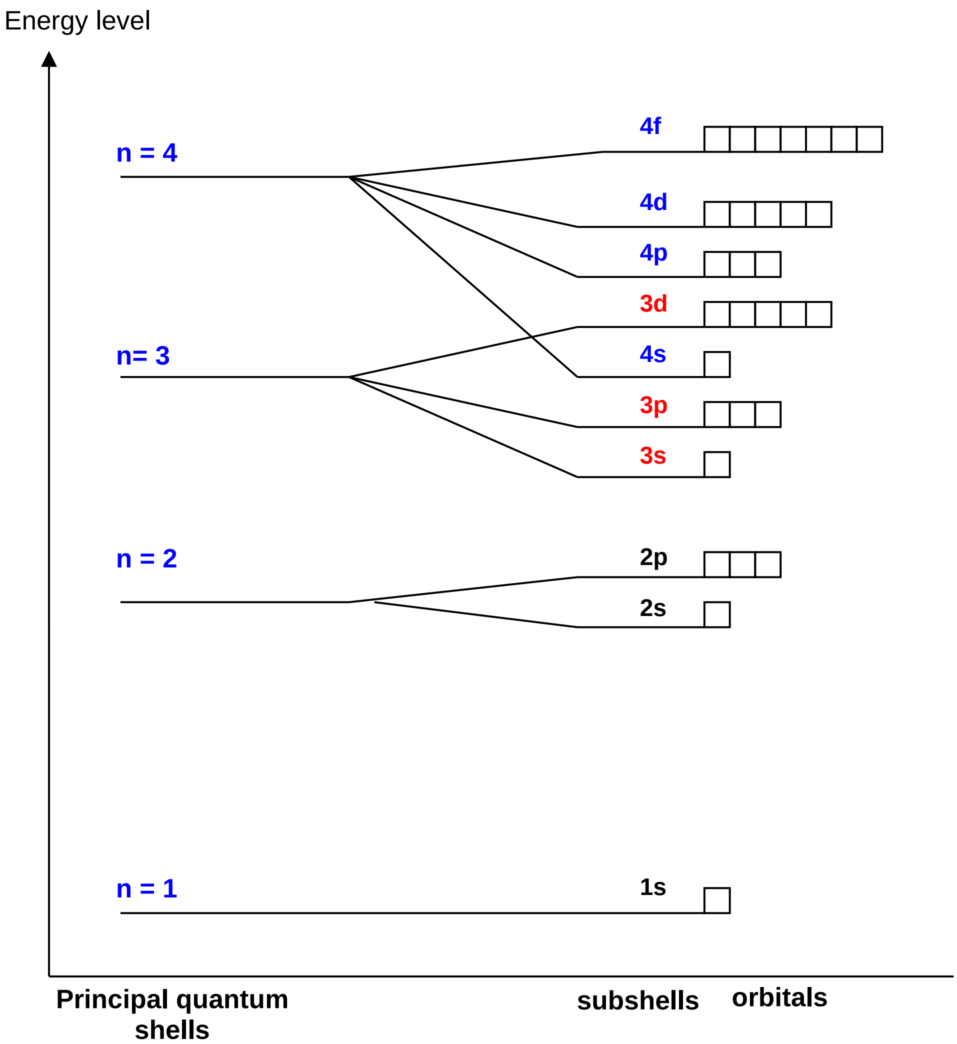
**Relative energy follows this order: s < p < d < f**

**Note:**
Energy level decreases with increasing probability of electrons found nearer to the nucleus.

Due to the shapes of the s, p and d orbitals, electrons in s orbitals have a higher probabilty of being found closer to the nucleus than electrons in the p orbitals, and the electrons in p orbitals have a higher probability of being found closer to the nucleus than electrons in the d orbitals.

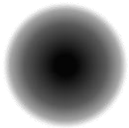
As n increases, the energy levels come **closer** to each other. As a result, overlapping of subshells of different principal quantum shell occur. The first overlap occurs between the **3d and the 4s subshells**.

**Video:**
Click on this to have a visual idea of the relative energy of the orbitals.



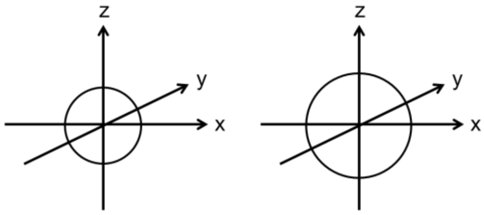
## 3.3 Shapes of Orbitals

**Note:**
Shape: <u>**spherical**</u>, non–directional



***s orbitals*** [There is only <u>**one**</u> orbital in the s subshell]

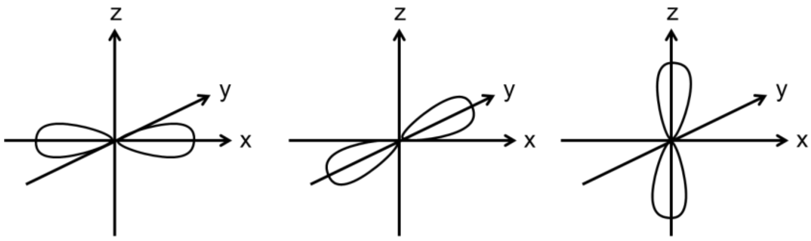
Size of s orbitals <u>increases</u>, as *n* increases → orbitals get bigger and more diffused i.e. lower probability of finding electrons very close to the nucleus.




1s orbital 2s orbital

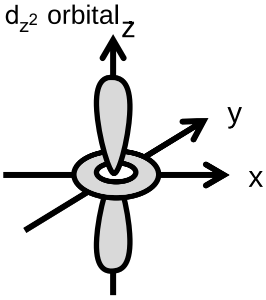
**Note:**
Shape: <u>dumb–bell</u>

***p orbitals*** [There are <u>**three**</u> different types of p orbitals ($p_x$, $p_y$, $p_z$)]
Size of p orbitals <u>increases</u> as *n* increases.




$p_x$ orbital $p_y$ orbital $p_z$ orbital

**Note:**
The actual representation of $d_{z^2}$ orbital



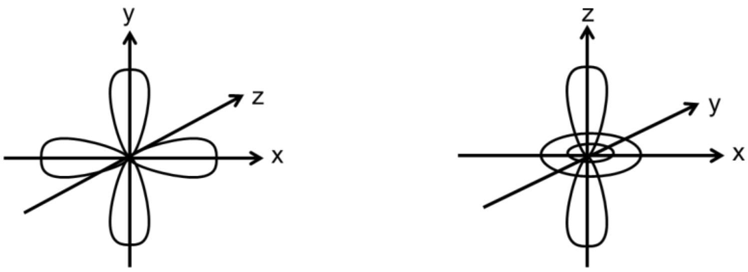

The lobes of $d_{x^2-y^2}$ lie along the x and y axes.

The lobes of $d_{xy}$, $d_{xz}$, $d_{yz}$ orbitals lie between the respective axes.

**Note:**
Orbitals in the same subshell are degenerate (same energy)

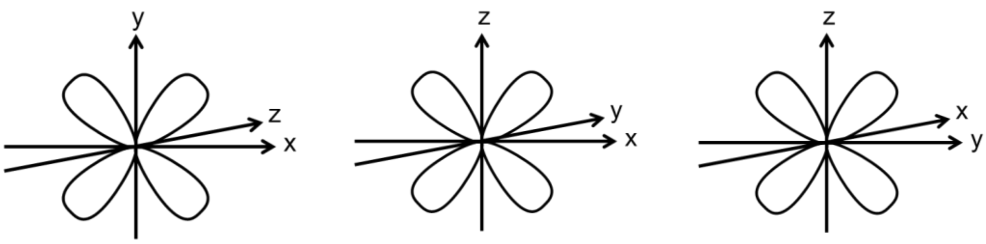
Size of orbital increases with n

***d orbitals*** [There are a total of <u>**five**</u> d-orbitals in each d-subshell]
Two of the orbitals ($d_{x^2-y^2}$, $d_{z^2}$) have electron density concentrated <u>**along**</u> the x, y and z axes.




$d_{x^2-y^2}$ orbital $d_{z^2}$ orbital

The other three orbitals ($d_{xy}$, $d_{xz}$, $d_{yz}$) have electron density concentrated <u>**between**</u> the x, y and z axes.




$d_{xy}$ orbital $d_{xz}$ orbital $d_{yz}$ orbital

**Checkpoint 3 (Think-pair-share)** 

1 Discuss if each statement is true (T) or false (F). Provide an explanation for statement that false.

(a) **There are two 2s orbitals.** **T / F**

Explanation (if any):

(b) **1s subshell and 2s subshell are in the same principal quantum shell.** **T / F**

Explanation (if any):

(c) **$3p_x$ orbital is at a higher energy level than $2p_x$ orbital.** **T / F**

Explanation (if any):

(d) **$3p_x$ orbital is at a higher energy level than $3p_y$ orbital.** **T / F**

Explanation (if any):

(e) **$2p_y$ and $3p_y$ orbitals have the same shape but different in size.** **T / F**

Explanation (if any):

(f) **3s, 3p and 3d orbitals are in the same subshell.** **T / F**

Explanation (if any):

(g) **Electrons orbit around the nucleus.** **T / F**

Explanation (if any):

# 4 ELECTRONIC CONFIGURATIONS

**Success criteria:**
- Able to give the ground state electronic configuration of atoms and ions with reference to the periodic table.

## 4.1 Ways to represent electronic configurations

Electronic configuration of an atom shows how electrons are arranged in the various orbitals.

| | Electronic configuration of Argon |
|---|---|
| Previously learnt | 2, 8, 8 |
| 'A' Level | $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^6$ |

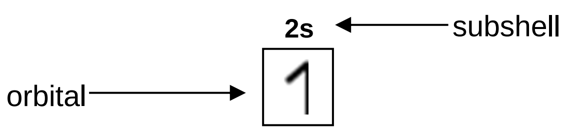
In 'A' level syllabus, electronic configurations can be represented in 2 ways:

1. In terms of **s, p, d, f** notations
   Principal quantum number is written, followed by the type of subshell. The number of electrons present in the given subshell is written as a superscript.

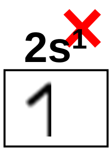
Principal quantum number, ***n*** = 2 → $2s^1$ ← 1 electron; ← s subshell

2. In terms of **electron-in-boxes** representation

   Each orbital is denoted by a box, and the electron is shown in the box as a half arrow (↿).



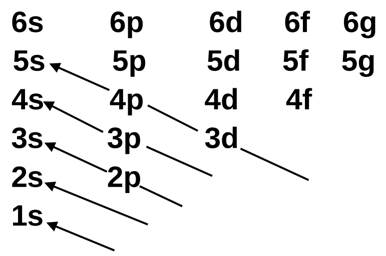

**Note:**
Do not include the number of electrons as the superscript of the subshell label. The example below is not accepted.



### 4.2 Rules to writing electronic configurations

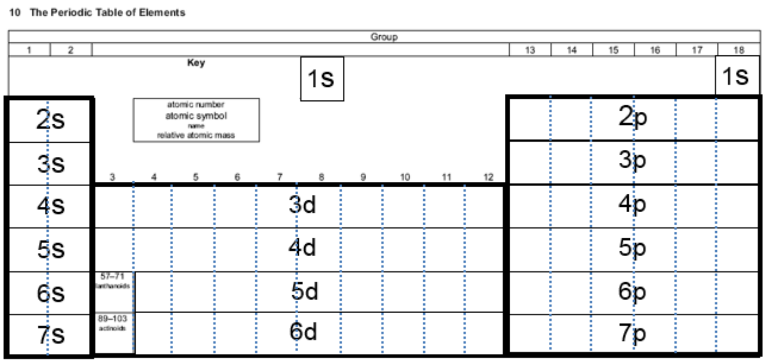
There are 3 rules which determine the order in which the electrons fill the vacant orbitals in an atom.

**Rule 1:**
***Aufbau Principle***
The added electron will occupy the empty orbital with the lowest energy first.




The order in which the orbitals are being filled is reflected in the Periodic Table.

**Note:**
After 3p orbitals are filled, 4s orbital is filled **BEFORE** 3d orbitals.



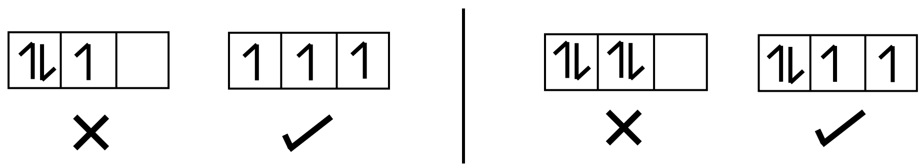

A new period starts when electrons enter a new principal quantum shell.
**Period number** refers to the **principal quantum number**, ***n***, of electrons in the valence (outermost) shell.

Elements in the **same Group have the similar valence shell electronic configuration**.

**Rule 2:** ***Hund's Rule***

When filling up a subshell, there is less inter-electron repulsion if each of the orbitals is occupied **singly** (i.e. half-filled) first before pairing occurs (i.e. before any single orbital is completely filled).

*Thus,*



**Rule 3:** ***Pauli Exclusion Principle***

An orbital can accommodate a maximum of two electrons of **opposite spins.**

" ↿ " represents one direction of spin while " ⇂ " represents the other direction.

Thus, [↿⇂] or [⇃↾] are correct while [↿↾] and [⇃⇂] are incorrect.

A species (atom or ion) is in the **ground state** when all its electrons occupy the **lowest energy levels**. When an electron receives energy and is promoted to a **higher energy level**, the species become unstable and is said to be in an **excited state**.

**Example:** ${}_{8}O$ atom
**Ground state** electronic configuration is $1s^2\ 2s^2\ \mathbf{2p^4}$.

An example of an **excited state** electronic configuration may be $1s^2\ 2s^2\ \mathbf{2p^3\ 3s^1}$.

### 4.3 Anomalous ground state electronic configurations for Cr and Cu

${}_{24}Cr$ is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{3d^5\ 4s^1}$ **NOT** $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{3d^4\ 4s^2}$

$\mathbf{3d^5\ 4s^1}$ electronic configuration is more stable than $\mathbf{3d^4\ 4s^2}$.

${}_{29}Cu$ is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{3d^{10}\ 4s^1}$ **NOT** $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{3d^9\ 4s^2}$

$\mathbf{3d^{10}\ 4s^1}$ electronic configuration is more stable than $\mathbf{3d^9\ 4s^2}$.

### 4.4 Nobel Gas Configuration

For atoms in Period 2 onwards, it is sometimes more convenient to represent their electronic configuration in a condensed form.

In writing the condensed electronic configuration of an element, the electronic configuration of the nearest noble gas element of lower atomic number is represented by its chemical symbol in brackets.

Example: ${}_{3}Li$ : [He] $2s^1$

Contains **inner core electrons** Contains valence shell electrons

**Note:**

The condensed configuration is more for conceptual understanding.

The **inner core electrons** do not take part in reaction.

Always write **full** electronic configuration in A level assessment.

Always write the electronic configuration in the **order in increasing n**.

e.g. For d block element:
…..$3d^{1-10}\ 4s^2$ **NOT** …$4s^2 3d^{1-10}$

## Checkpoint 4(a)

**1 Complete the table below with reference to the periodic table.**

| In terms of **s, p, d, f** notations | |
|---|---|
| | Full electronic configuration |
| $_{1}H$ | $1s^{1}$ |
| $_{2}He$ | $1s^{2}$ |
| $_{3}Li$ | $1s^{2}\ 2s^{1}$ |
| $_{4}Be$ | |
| $_{5}B$ | |
| $_{6}C$ | |
| $_{7}N$ | |
| $_{8}O$ | |
| $_{9}F$ | |
| $_{10}Ne$ | |
| $_{19}K$ | |
| $_{20}Ca$ | |
| $_{22}Ti$ | |
| *$_{24}Cr$ | $1s^{2}\ 2s^{2}\ 2p^{6}\ 3s^{2}\ 3p^{6}\ 3d^{5}\ 4s^{1}$ |
| *$_{29}Cu$ | $1s^{2}\ 2s^{2}\ 2p^{6}\ 3s^{2}\ 3p^{6}\ 3d^{10}\ 4s^{1}$ |

| **electron-in-boxes** representation | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1s | 2s | 2p | | | 3s | 3p | | | 3d | | | | | 4s |
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## Checkpoint 4(b) 

**1** Which atom has 2 unpaired electrons?

**A** Ba
**B** Ge
**C** Fe
**D** Sc

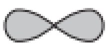
( )

**2** Which atom has a half-filled set of 4p electrons?

**A** A*l*
**B** P
**C** Ga
**D** As

( )

**3** The table refers to the electron distribution in the second shell of an atom with eight protons. Which row is correct for this atom?

| | Orbital shape  | | Orbital shape  | |
|---|---|---|---|---|
| | Orbital type | Number of electrons | Orbital type | Number of electrons |
| **A** | p | 2 | s | 4 |
| **B** | p | 4 | s | 2 |
| **C** | s | 2 | p | 4 |
| **D** | s | 4 | p | 2 |

( )

**5** Using the ground state valence electronic configuration of atom given below, **i**dentify the elements with reference to the periodic table.

(i) $4s^2 4p^4$
(ii) $5s^2 5p^1$

### 4.5 Writing Electronic Configurations for ions

**1.** Write the electronic configuration of the atom first.

**2.** For **cation**, remove electron(s) from outermost shell.
(remove electrons from **4s** before **3d**)
For **anion**, add electron(s) to outermost shell.

**Video:**
Click on this to review the order of writing electronic configuration.

***Worked example 2***

i) Write the electronic configuration for $_{16}S^{2-}$.

*Step 1: electronic configuration for $_{16}S$*
**$1s^2 2s^2 2p^6 3s^2 3p^4$**

*Step 2: For anion, add electron to the outermost shell.*
**Hence electronic configuration for $_{16}S^{2-}$ : $1s^2 2s^2 2p^6 3s^2 3p^6$**

ii) Write the electronic configuration for $_{11}Na^{+}$.

*Step 1: electronic configuration for $_{11}Na$*
**$1s^2 2s^2 2p^6 3s^1$**

*Step 2: For cation, remove electron from the outermost shell.*
**Hence electronic configuration for $_{11}Na^{+}$: $1s^2 2s^2 2p^6$**

iii) Write the electronic configuration for $_{26}Fe^{2+}$.

*Step 1: electronic configuration for $_{26}Fe$*
**$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$**

*Step 2: For cation, remove electron from the outermost shell (remove $e^-$ from 4s before 3d).*
**Hence electronic configuration for $_{26}Fe^{2+}$: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$**

**Checkpoint 5**

1. Write the electronic configuration and draw the electron-in-boxes representation to represent the electronic configurations of each of the following species.

(a) $_{15}P^{3-}$

1s 2s 2p 3s 3p

(b) $_{24}Cr^{+}$

1s 2s 2p 3s 3p 3d

**Success criteria:**
- Explain the factors influencing the successive ionisation energies of a particular element.
- Deduce the group number of an element from its successive ionisation energy data.

## 5 IONISATION ENERGY

**The first ionisation energy** of an element is the **energy required** to remove **<u>1 mole</u> of most loosely held electrons** from **<u>1 mole</u> of <u>gaseous atoms of the element</u>** to form **<u>1 mole</u>** of **<u>singly-charged gaseous cations</u>**.

Eqn: $X(g) \rightarrow X^{+}(g) + e^{-}$ $\Delta H$ = positive

**Note:**
State symbols <u>must</u> be included in the equation as a different state would mean a different amount of energy involved.

**The second ionisation energy** of an element is the energy required to remove **<u>1 mole</u>** of most loosely held electrons from **<u>one mole</u>** of **<u>singly positive charged gaseous cations ($X^{+}$)</u>** to form **<u>one mole</u>** of **<u>doubly charged gaseous cations ($X^{2+}$)</u>**

Eqn: $X^{+}(g) \rightarrow X^{2+}(g) + e^{-}$ $\Delta H$ = positive

All ionisation energies are <u>endothermic (+ve)</u> as **energy** is **required** to overcome the **attraction** between the **nucleus** and the **electron** to be removed.

Generally for the **n$^{th}$ IE**:

$X^{(n-1)+}(g) \rightarrow X^{n+}(g) + e^{-}$ $\Delta H$ = positive

**<u>Checkpoint 6</u>** 

Write the equations that represent the 1st and 2nd ionisation energies of C*l*.

### 5.1 Successive ionisation energies

**Successive** ionisation energies always **increase**.

1st IE < 2nd IE < 3rd IE < 4th IE < …

This is because

the **number of protons** exerting nuclear attraction on the electrons remains the **same**.

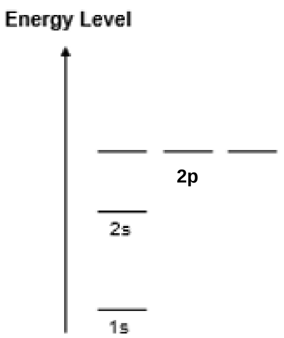
while the **number of remaining electrons decreases** with the progressive removal of electron **from the same element.**

The **group number** in the Periodic Table can be deduced from its successive ionisation energy data.

**Plots of successive IEs of an element**

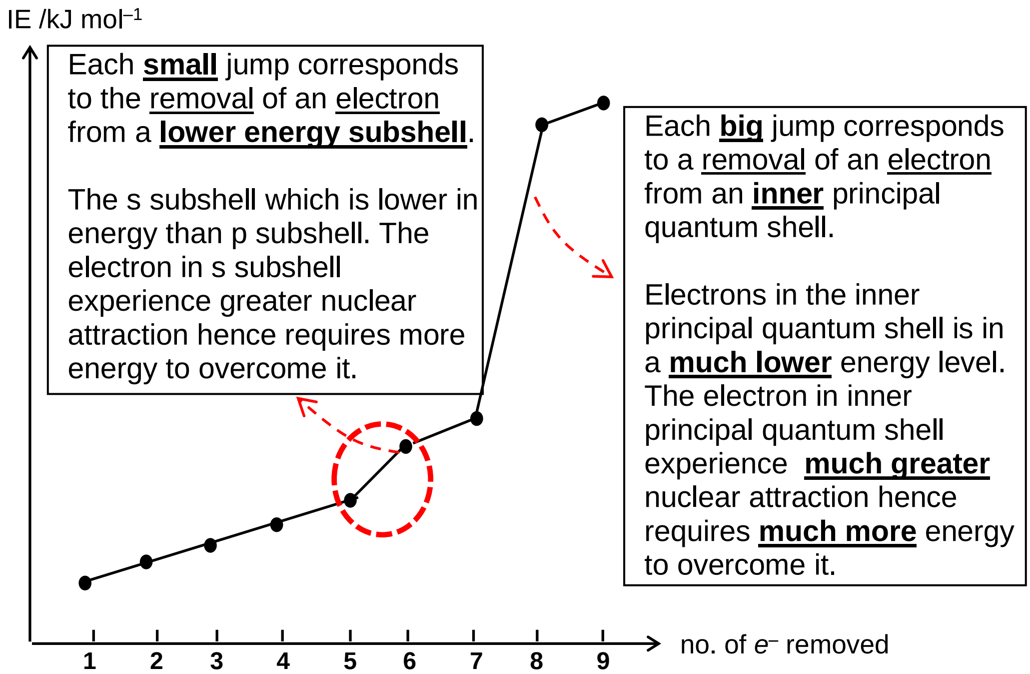
**Note:**
Nuclear attraction = (electrostatic forces of attraction between the nucleus and the valence electrons)

The relative energy level of the subshells/orbitals in the atom




The graph below shows all the successive ionisation energies of fluorine (atomic number = 9).

Electronic configuration of F: <u>**$1s^2$ $2s^2$ $2p^5$**</u>




**Observations:**

1. Gradual increase in IEs when successive electrons are removed from the same subshell.

2. Small jump IE when successive electron is removed from a lower energy subshell of the same principal quantum shell. (5th to 6th IE)

3. Big jump in IE when successive electron is removed from an inner principal quantum shell. (7th to 8th IE)

### 5.2 Using successive IEs to determine the group number of an atom

Successive IEs can be used to deduce the electronic configuration of an element and hence, the position of that element in the Periodic Table.

***Worked Example 3***

The first seven IEs of an element **X** are as follows:

870 1800 3000 3600 5800 7000 13000 / kJ mol$^{-1}$

State, giving reasons, the group of the Periodic Table to which **X** is likely to belong.

The **big jump** in the I.E. is from the **6th to 7th**, implying the **7th electron** is removed from the **inner principal quantum shell**. Hence there are **6 valence electrons**.
**X** is in group **16**.

**Checkpoint 7** 

**1** The first seven successive ionisation energies (in kJ mol$^{-1}$) of an element **J** are given below:

1020 1950 2730 4580 6020 12300 15400

Deduce which Group does element **J** belongs to? Write down the valence shell electronic configuration of element **J**.

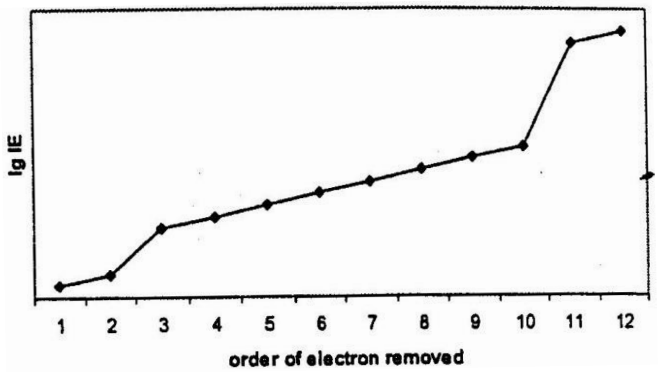
**Checkpoint 7 (Continued)**

**2** The table below shows the first 8 successive IEs (in kJ $mol^{-1}$) for elements **Y** and **Z**.

| | $1^{st}$ | $2^{nd}$ | $3^{rd}$ | $4^{th}$ | $5^{th}$ | $6^{th}$ | $7^{th}$ | $8^{th}$ |
|---|---|---|---|---|---|---|---|---|
| **Y** | 578 | 1817 | 2745 | 11577 | 14842 | 18379 | 23326 | 27465 |
| **Z** | 1012 | 1907 | 2914 | 4937 | 6274 | 21267 | 25431 | 29872 |

Deduce which groups in the Periodic Table does each element, **Y** and **Z,** belong to?

**3** The diagram below shows successive ionisation energy values of all electrons for an unknown element **Z**.




**(a)** Account for the large difference between the $2^{nd}$ and $3^{rd}$ ionisation energy values.

**(b)** How many occupied principal quantum shells does **Z** have?

**(c)** Write the electronic configuration of **Z.**

# APPENDIX

**Four new elements added to periodic table: 5 things about the chemistry chart**
*By Lee Min Kok* PUBLISHED JAN 6, 2016, 1:28 PM SGT

Still using an old science textbook? It's time to get a new one then, after four new super-heavy elements were added to the periodic table recently.

The International Union of Pure and Applied Chemistry (IUPAC), the US-based global authority on chemistry, had announced on Dec 30 last year that the table's seventh row was now complete. Elements 113, 115, 117 and 118 were added to the table - its first update since 2011 - and will be named in the coming months by the scientific teams who discovered them. They will be known temporarily by their working names of ununtrium (Uut or 113), ununpentium (Uup or 115), ununseptium (Uus or 117), and ununoctium (Uuo or 118).

All four are synthetic and were discovered by slamming light nuclei into each other and tracking the decay of radioactive super-heavy elements (which exist only very briefly before decaying into other elements), reported The Guardian. IUPAC awarded the discovery of element 113 to a team of scientists from Japan's Riken Institute after they successfully created it three times between 2004 and 2012. It will be the first element on the table to be named in Asia.

The discovery of the other three elements were claimed by a Russian-American team from the Joint Institute for Nuclear Research in Dubna, the Oak Ridge National Laboratory in Tennessee and the Lawrence Livermore National Laboratory in California.

With the periodic table now looking complete - till its next update, at least - here are some interesting facts about the universal chart used by scientists, teachers and students.

***Who Came Up With The Table?***

Although several scientists had been known to present their own tables earlier, Russian chemist Dmitri Mendeleev's version - a list arranged in order of the elements' increasing atomic weight - was the first to gain widespread acceptance among the scientific community in 1869. The modern day version of the table, however, is organised in a grid system and orders the elements by increasing atomic number.

### *How Do You Read The Table?*

There are seven rows, called periods, and 18 columns, called groups, in the table. Elements in the same group share similar properties. Those in the same period have the same number of atomic orbitals (the wave-like behaviour of either one or a pair of electrons in an atom) - for instance, the first period only has two elements, hydrogen and helium, with only a single orbital.

Most elements on the table are metals divided into six broad categories - alkali metals, alkaline earths, basic metals, transition metals, lanthanides and actinides. They are located on the left, separated from the non-metals on the right by a zig-zag line. Lanthanides and actinides, often called "inner transition metals", are commonly hived off as a separate section under the main table as including all 30 - including Uranium - would make the table too wide.
The table is a useful tool for people to derive relationships between the different properties of the elements. It can also help predict the properties of new elements that have yet to be discovered or created.

### *How Many Elements Are There?*

Currently, there is only room for 118 elements. Of the 118, 90 - 1 through 92, with the exception of elements 43 (Technetium, Tc) and 61 (Promethium, Pm) - occur naturally on Earth, although some are extremely rare and can only be found in small quantities. The rest are synthetic. Technetium was the first element to be made artificially; the silvery grey metal was found in 1936 as part of an experiment conducted in an Italian university. An eighth period could be added to the table once elements 119 (Ununennium) and 120 (Unbinilium) have been verified. Attempts to synthesise both elements have been unsuccessful thus far.

### *How Are New Elements Named?*

According to the IUPAC, new elements can be named after a mythological concept, a mineral, a place or country, a property or a scientist. After initial acceptance, the element's name and two-letter symbol are put up for public review for five months before the IUPAC Council makes its final decision. The element Einsteinium (Es), discovered in 1952, was named in honour of renowned scientist Albert Einstein, while Europium (Eu) is named after the continent of Europe after it was isolated in 1901. Thorium (Th) gained its name from Thor, the Norse God of Thunder, upon its discovery in 1828. It is currently being used as a nuclear fuel due to its radioactivity. The Riken Institute had earlier said that the name Japonium (in honour of Japan) might be proposed for element 113.

### *When Were New Elements Last Added To The Table?*

The table's last major revision occurred in June 2011, when elements 114 and 116 were also discovered by a joint Russian-American team from Dubna's Joint Institute for Nuclear Research and California's Lawrence Livermore National Laboratory. Their names were ratified by the IUPAC nearly a year later on May 30, 2012 - element 114 became known as Flerovium (Fl) and element 116, Livermorium (Lv). Both are highly radioactive and were the heaviest elements on the table until the recent discovery of elements 115, 117 and 118.

***Sources: International Union of Pure and Applied Chemistry website, AFP, BBC, Chemistry.about.com***

| Success criteria: | Relevant Tutorial questions | What do you still struggle with? Write your queries here. |
|---|---|---|
| 1. Identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses. | DQ 6, 11 | |
| 2. Define nucleon number (mass number) and proton number (atomic number). | DQ 1/2/5 | |
| 3. Deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge). | | |
| 4. Recognise that only the proton number determines the chemical identity of an atom. | DQ 2-5 | |
| 5. Able to deduce the direction of subatomic particles (protons, neutrons and electrons) and charged particles in an electric field. | DQ 6 | |
| 6. Able to compare the angle of deflection by considering their $\frac{charge}{mass}$ ratio. | | |
| 7. Able to define terms relative atomic mass and relative isotopic mass. | DQ 7 | |
| 8. Able to calculate the relative atomic mass of an element given the relative abundances of each isotope. | DQ 5 | |
| 9. 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. | DQ 8 | |
| 10. Able to draw the s, p and d orbitals on x, y and z axis, showing their shapes and orientation in space accurately. | DQ 14 | |
| 11. Able to describe the shapes of s and p orbitals and recognize that their size increases with n. | DQ 5 | |
| 12. Able to give the ground state electronic configuration of atoms and ions with reference to the periodic table. | DQ 9, 10, 11, 12, 13 | |
| 13. To show understanding of what successive ionisation of a particular element mean. | DQ 15 | |
| 14. Explain the factors influencing the successive ionisation energies of a particular element. | DQ 16, 17 | |
| 15. Deduce the group number of an element from its successive ionisation energy data. | DQ 16, 17 | |

# Tutorial – Atomic Structure

## Discussion Questions

### Atomic Number and Mass Number

**1.** *Use of the Data Booklet is relevant to this question.*

Nuclear magnetic resonance (NMR) spectroscopy is an analytical technique that uses the magnetic properties of certain atomic nuclei in order to elucidate the structure of an organic molecule.

Atomic nuclei with an even number of protons and an odd number of neutrons (or vice versa) are most suitable for NMR spectroscopy.

Which of the following nuclei is **least** suitable for NMR spectroscopy?

**A** $^{28}Si$ **B** $^{31}P$ **C** $^{103}Rh$ **D** $^{19}F$

**2** *Use of the Data Booklet is relevant to this question.*

Tritium, $^{3}_{1}H$, a radioactive isotope of hydrogen, slowly turns into a helium isotope $^{3}_{2}He$.

Which statements about the two isotopes are **incorrect**?

**1** Both isotopes have more neutrons than electrons.

**2** Both isotopes have the same number of protons in their nuclei.

**3** Both isotopes have the same number of charged sub–atomic particles.

**A** 2 only
**B** 1 and 3 only
**C** 2 and 3 only
**D** 1, 2 and 3

**3** Some isotopes are unstable and undergo nuclear (radioactive) reactions. In one type of reaction, an unstable nucleus assimilates an electron from an inner orbital of its electron cloud. The net effect is the conversion of a proton and an electron into a neutron.

Which of the following describes this type of reaction?

**A** $^{11}C \rightarrow {}^{12}C$
**B** $^{111}I \rightarrow {}^{111}Te$
**C** $^{76}Br \rightarrow {}^{75}Br$
**D** $^{76}Kr \rightarrow {}^{75}Br$

A level 2015 P3 Q5

**5** Lithium metal and its compounds have many uses, ranging from nuclear chemistry, rechargeable batteries, organic reagents and pharmaceuticals.

(a) *Naturally occurring* lithium contains isotopes $^{6}Li$ and $^{7}Li$.

**(i)** What is meant by the terms

- proton number,
- nucleon number? [1]

**(ii)** The isotopes $^{6}Li$ and $^{7}Li$ have accurate isotopic mass of 6.015 and 7.016 respectively.

The $A_r$ of lithium is 6.942.

Calculate the relative percentage abundances of the two isotopes, to **two** decimal places.

[2]

**(iii)** A nuclear reaction is a reaction in which there is a change to an atomic nucleus.

An experimental nuclear reactor uses $^{6}Li$ and deuterium, $^{2}H$, as fuel. Three nuclear reactions between these two atoms are described below ($P^{+}$ is a proton; n is a neutron).

$$^{6}Li + {}^{2}_{1}H \rightarrow 2\,^{4}He$$

$$^{6}Li + {}^{2}_{1}H \rightarrow {}^{4}He + \mathbf{X} + n$$

$$^{6}Li + {}^{2}_{1}H \rightarrow \mathbf{Y} + P^{+}$$

Suggest the identities of **X** and **Y**.

[2]

**6** Beams of charged particles are deflected by an electric field. When a beam of protons passes through an electric field of constant strength, the angle of deflection is +12 °.

In another experiment under identical conditions, particle Y is deflected by an angle of – 4 °.

What could be the composition of particle Y?

| | protons | neutrons | electrons |
|---|---|---|---|
| 1 | 1 | 2 | 2 |
| 2 | 3 | 3 | 5 |
| 3 | 4 | 5 | 1 |

**A** 1, 2 and 3 **B** 1 and 2 **C** 1 only **D** 3 only

A level 2011 P1 Q31

**7** Which statement about relative molecular mass are correct?

**1** It is the sum of the relative atomic masses of all the atoms within the molecule.

**2** It is the ratio of the average mass of a molecule to the mass of a $^{12}C$ atom.

**3** It is the ratio of the mass of 1 mol of molecules to the mass of 1 mol of $^{1}H$ atoms.

**A** 1, 2 and 3 **B** 1 and 2 only **C** 2 and 3 only **D** 1 only

**Electronic Configuration**

**8** Gallium has the electronic configuration [Ar] $3d^{10}4s^{2}4p^{1}$, where [Ar] represents the electronic configuration of argon. In which order are the electrons lost in forming the $Ga^{4+}$ ion?

**A** 3d, 4p, 4s, 4s **B** 4s, 4s, 4p, 3d **C** 4p, 3d, 3d, 3d **D** 4p, 4s, 4s, 3d

**9** An isolated gaseous species has paired electrons in at least one of its 3d orbitals and a fully filled 4s subshell.

What could be the identity of the species?

**A** Cu **B** $Fe^{3+}$ **C** $Ni^{2+}$ **D** $Sr^{2+}$

**10** Which ion has the most number of unpaired electrons?

**A** $Cr^{3+}$ **B** $Ni^{2+}$ **C** $Ca^{2+}$ **D** $Co^{3+}$

**11** *Use of the Data Booklet is relevant to this question.*

What do the ions $^{23}Na^{+}$ and $^{24}Mg^{2+}$ have in common?

**A** Both ions have more electrons than neutrons.
**B** Both ions have 12 neutrons in their nuclei.
**C** Both ions contain the same number of nucleons in their nuclei.
**D** Both ions have an outer electronic configuration of $3s^{2}\,3p^{6}$.

**12** A stable ion of **Q** has the following properties:

- has a noble gas configuration
- was obtained by removing electrons from the same orbital

Which could be **Q**?

**A** A*l* **B** Ca **C** Cu **D** S

**13** Write the *ground state* electronic configuration of

**(a)** S atom
**(b)** $O^+$ ion
**(c)** $Cl^-$ ion
**(d)** Cu atom
**(e)** $Fe^{3+}$ ion
**(f)** Ge atom

**14** Describe the shapes of all the orbitals occupied by electrons in Manganese atom, $_{25}Mn$.

**Successive Ionisation Energy**

**15** *Use of the Data Booklet is relevant to this question.*

The electronic configuration of four elements are given.

Which element will most easily form an isolated gaseous ion with the charge of 3+?

**A** $1s^2 2s^2 2p^3$
**B** $1s^2 2s^2 2p^6 3s^2 3p^3$
**C** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
**D** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$

**16** The successive ionisation energies of two elements, **M** and **N**, are given.

| Ionisation energy / kJ mol$^{-1}$ | 1st | 2nd | 3rd | 4th | 5th | 6th | 7th | 8th |
|---|---|---|---|---|---|---|---|---|
| **M** | 1090 | 2350 | 4610 | 6220 | 37800 | 47000 | - | - |
| **N** | 1251 | 2298 | 3822 | 5158 | 6542 | 9362 | 11018 | 33604 |

What is the formula of the compound that **M** and **N** are likely to form?

**A** **MN** **B** $\mathbf{M_2N_2}$ **C** $\mathbf{MN_4}$ **D** $\mathbf{M_4N}$

**17** The successive ionisation energies (I.E.) of two elements, **Q** and **R**, are shown below:

| **IE / kJ mol$^{-1}$** | **1st** | **2nd** | **3rd** | **4th** | **5th** | **6th** | **7th** | **8th** |
|---|---|---|---|---|---|---|---|---|
| **Q** | 1000 | 2252 | 3357 | 4556 | 7004 | 8496 | 27107 | 31719 |
| **R** | 578 | 1817 | 2745 | 11577 | 14842 | 18379 | 23326 | 27465 |

What is the likely formula of the compound formed when **Q** and **R** reacts together?

**A** $\mathbf{Q_3R_2}$ **B** $\mathbf{Q_2R_3}$ **C** $\mathbf{QR_3}$ **D** $\mathbf{Q_3R}$