Unit 2

# Structure of Atom

- The word atom is a Greek word meaning indivisible. According to Dalton's atomic theory, atom is the smallest indivisible part of matter which takes part in chemical reactions. In 1833, Michael Faraday showed that there is a relationship between matter and electricity. The discovery of electrons, protons and neutrons discarded the indivisible nature of atom proposed by John Dalton.

## Atomic Number ($Z$)

- Atomic number of an element is the number of positive charges (or the number of protons, $p$) present in the nucleus of the atom.
- Since the atom as a whole is electrically neutral, therefore the number of positively charged particles *i.e.* protons present in the atom must be equal to the number of negatively charged particles *i.e.* electrons present in it.
- Atomic number of an element
  = total number of protons present in the nucleus
  = total number of electrons present in the atom.

## Mass Number ($A$)

- The total mass of an atom is mainly due to protons and neutrons, and the sum of the number of protons and neutrons (nucleons) in the nucleus of the atom is known as mass number.
- $A = Z + N$, where $N$ is the number of neutrons. An element $X$ having a mass number $A$ and atomic number $Z$ is represented as:

$$_{Z}X^{A} \text{ or } {}^{A}_{Z}X$$

## Isotopes

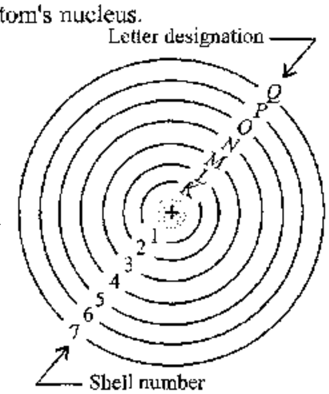
- Isotopes are the atoms of the same element having different atomic masses. *e.g.* ${}^{1}_{1}H$, ${}^{2}_{1}H$ and ${}^{3}_{1}H$.
- Isotopes of an element possess identical chemical properties but differ slightly in physical properties.
- Number of neutrons present in the nuclei of various isotopes of an element is always different.
- All the isotopes of an element occupy the same position in the periodic table.

## Isobars

- These are the atoms of different elements having same mass number but different atomic numbers.
  *e.g.* ${}^{40}_{19}K$ and ${}^{40}_{20}Ca$, ${}^{14}_{6}C$ and ${}^{14}_{7}N$, etc.
- Number of electrons or protons (atomic number) is different but the sum of number of neutrons and protons (mass number) is same.
- Isobars occupy different positions in periodic table.
- Because these are atoms of different elements so their chemical properties are different but as their atomic masses are same so they possess almost identical physical properties.

## CONCEPTS OF SHELLS AND SUBSHELLS

- An electron shell may be thought of as an orbit followed by electrons around an atom's nucleus.
- The electron shells are labelled as $K, L, M, N, O, P$ and $Q$; or 1, 2, 3, 4, 5, 6 and 7 ; going from innermost shell to outwards.
- Each shell can contain only a fixed number of electrons, the $n$ shell to can hold up to $2n^2$ electrons.
- The electrons in outer shell have higher average energy and travel farther from nucleus than those in inner shells. Thus electrons of outer shells are more important for reactivity.

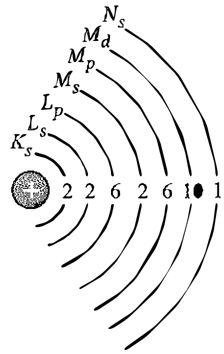


Shell designation in an atom

### Subshell

- Each shell consists of one or more subshells and each subshell consists of one or more atomic orbitals.
- There are four different types of subshells. These various subshells are denoted by letters $s$, $p$, $d$ and $f$.

| Shell name | Subshell name | Max. electrons in subshell | Max. electrons in shell |
|---|---|---|---|
| $K$ | $1s$ | 2 | 2 |
| $L$ | $2s$<br>$2p$ | 2<br>6 | 2 + 6 = 8 |
| $M$ | $3s$<br>$3p$<br>$3d$ | 2<br>6<br>10 | 2 + 6 + 10 = 18 |
| $N$ | $4s$<br>$4p$<br>$4d$<br>$4f$ | 2<br>6<br>10<br>14 | 2 + 6 + 10 + 14 = 32 |




Copper atom

- The subshell $s$ is of lowest energy and the $f$ subshell is of highest energy subshell.

## Dual Nature

- In 1924, deBroglie proposed that an electron, like light, behaves both as a material and as a wave. This proposal gave birth to wave mechanical theory which states that electrons, protons and even atoms when in motion possess wave properties.
- The de Broglie wavelength of a particle is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

where, $h$ = Planck's constant, $m$ = mass of particle
$v$ = velocity, $p$ = momentum

- Let kinetic energy of the particle of mass '$m$' is $E$.

$$E = \frac{1}{2}mv^2$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

## Modifications made by Davisson and Germer

- Davisson and Germer demonstrated the physical reality of the wave nature of electrons by showing that a beam of electrons could also be diffracted by crystals just like light of X-rays.

Let a charged particle, say an electron, be accelerated with a potential of $V$, then kinetic energy $1/2mv^2$ acquired by this electron due to the electric field shall be equal to the electrical force.

$$\frac{1}{2}mv^2 = eV$$

- According to de Broglie, $mv = \frac{h}{\lambda}$

$$\lambda = \frac{h}{\sqrt{2meV}}$$

## de Broglie Wavelength

| For charged particle | For uncharged particle |
|---|---|
| Electrons, $\lambda = \frac{12.27}{\sqrt{V}}$ Å | Neutrons, $\lambda = \frac{0.286}{\sqrt{E\text{ (eV)}}}$ Å |
| Proton, $\lambda = \frac{0.286}{\sqrt{V}}$ Å | Gas molecules, $\lambda = \frac{h}{\sqrt{3mkT}}$ |
| α-particles, $\lambda = \frac{0.101}{\sqrt{V}}$ Å | where, $k$ = Boltzmann constant |
| where, $V$ = accelerating potential of these particles | $E$ = kinetic energy |

### Illustration 1

The kinetic energy of an electron is $4.55 \times 10^{-25}$ J. Calculate the wavelength ($h = 6.6 \times 10^{-34}$ J sec, mass of electron $= 9.1 \times 10^{-31}$ kg).

**Soln.:** $K.E. = \frac{1}{2}mv^2 = 4.55 \times 10^{-25}$

or $\frac{1}{2} \times 9.1 \times 10^{-31} \times v^2 = 4.55 \times 10^{-25}$

or $v^2 = \frac{2 \times 4.55 \times 10^{-25}}{9.1 \times 10^{-31}}$ or $v = 10^3$ m s$^{-1}$

Applying de Broglie equation,

$$\lambda = \frac{h}{mv} = \frac{6.6 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^3} = 0.72 \times 10^{-6} \text{ m}$$

## Heisenberg's Uncertainty Principle

- Heisenberg's uncertainty principle implies that it is impossible to know simultaneously the position and velocity (or momentum) of a microscopic moving particle like electron, proton, etc.

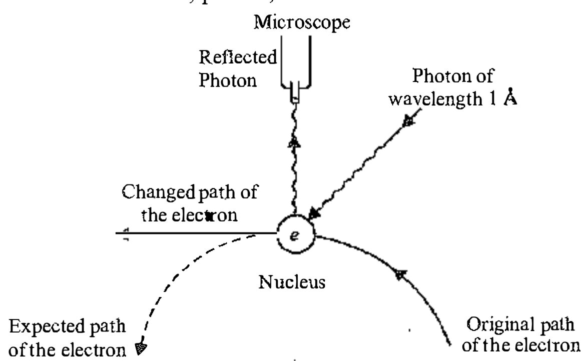



**Fig :** Change in the path and velocity of a moving electron by the impact of a photon of light of wavelength equal to 1 Å.

- **Mathematical relation :** If $\Delta x$ is the uncertainty in defining the position and $\Delta v$ is uncertainty in the velocity, the uncertainty principle may be expressed mathematically as,

$$\Delta x \cdot \Delta v \geq \frac{h}{4\pi}$$

### Illustration 2

A dust particle has mass equal to $10^{-11}$ g, diameter equal to $10^{-4}$ cm and velocity equal to $10^{-4}$ cm s$^{-1}$. The error in measurement of velocity is 0.1%. Calculate uncertainty in its position.

**Soln.:** $\Delta v = \frac{0.1 \times 10^{-4}}{100} = 1 \times 10^{-7}$ cm s$^{-1}$

$\because \quad \Delta v \cdot \Delta x = \frac{h}{4\pi m}$

$\therefore \quad \Delta x = \frac{6.626 \times 10^{-27}}{4 \times 3.14 \times 10^{-11} \times 1 \times 10^{-7}} = 5.27 \times 10^{-10}$ cm

The uncertainty in position as compared to particle size

$$= \frac{\Delta x}{\text{diameter}} = \frac{5.27 \times 10^{-10}}{10^{-4}} = 5.27 \times 10^{-6} \text{ cm}$$

## Atomic Orbital

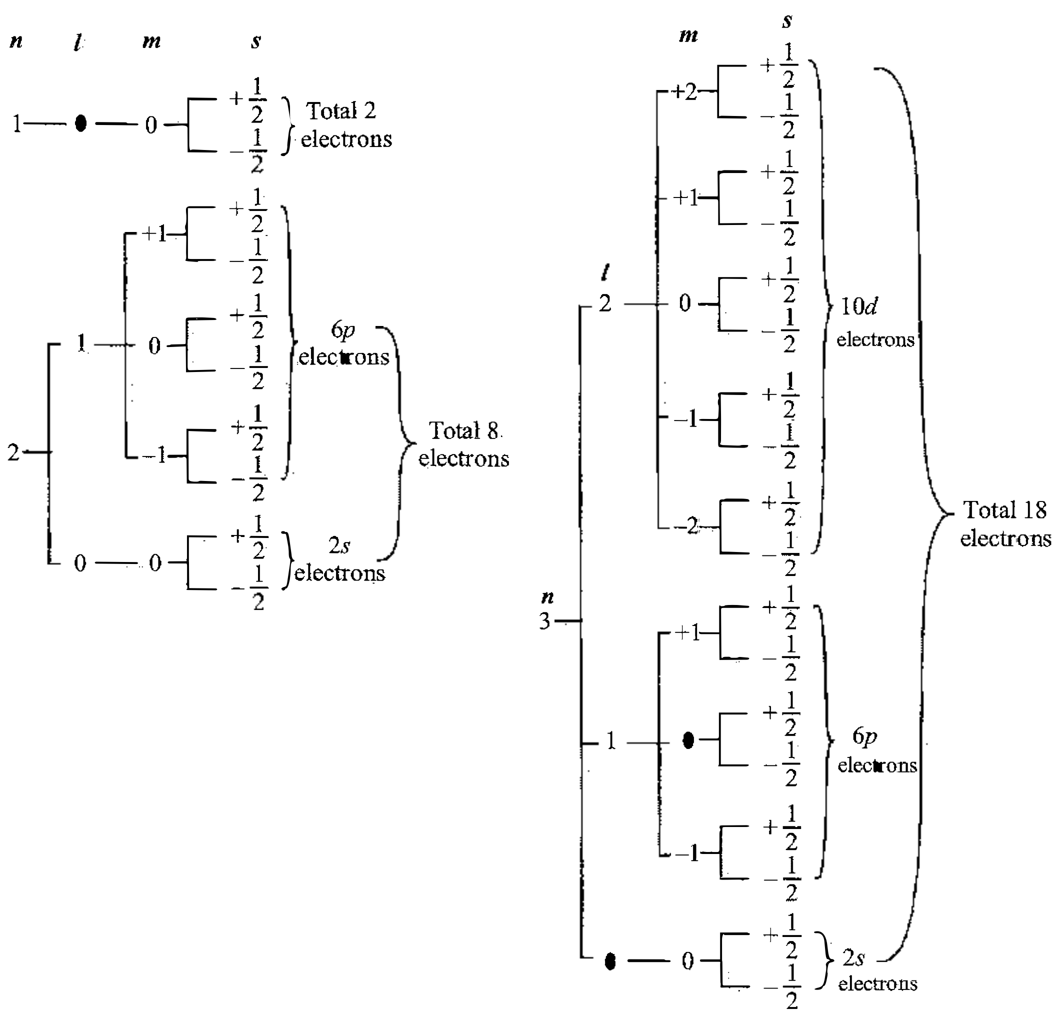
- The three dimensional space around the nucleus within which the probability of finding an electron of given energy is maximum, is called atomic orbital.

- Atomic orbital is the spatial description of the motion of an electron corresponding to a particular energy level. The energy of electron in an atomic orbital is always the same.

## Quantum Numbers

- It is defined as a set of four numbers which gives complete information about the electron in an atom *i.e.* energy, orbital occupied, size, shape and orientation of that orbital and the direction of electron spin.

| | Principal quantum number ($n$) | Azimuthal or angular quantum number ($l$) | Magnetic quantum number ($m$) | Spin quantum number ($s$) |
|---|---|---|---|---|
| **Used to** | specify the position and energy of electron. | describe orbital or subshell | determine the preferred orientations of orbitals in space. | account the spin of electrons. |
| **Values** | $n = 1, 2, 3, \ldots, \infty$ | $l = 0, 1, 2, \ldots (n-1)$ | $-l \ldots 0 \ldots +l$ | +1/2 or −1/2 |
| **Examples** | 1, 2, 3, 4, 5, 6, 7<br>*K L M N O P Q* | 0, 1, 2, 3<br>*s p d f* | | |
| **Used for calculating** | Minimum number of electrons = $2n^2$<br>$E_n = \dfrac{-13.6\,Z^2}{n^2}$ | Orbital angular momentum<br>$= \dfrac{h}{2\pi}\sqrt{l(l+1)}$<br>$s < p < d < f$ | Total value of $m = (2l+1)$<br>$s \Rightarrow m = 0$ (1 value)<br>$p \Rightarrow m = -1, 0, +1$ (3 values)<br>$d \Rightarrow m = \pm 2, \pm 1, 0$ (5 values)<br>$f \Rightarrow m = \pm 3, \pm 2, \pm 1, 0$ (7 values) | Spin angular momentum<br>$= \dfrac{h}{2\pi}\sqrt{s(s+1)}$<br>$s \Rightarrow$ maximum 2 electrons<br>$p \Rightarrow$ maximum 6 electrons<br>$d \Rightarrow$ maximum 10 electrons<br>$f \Rightarrow$ maximum 14 electrons |




Quantum numbers and the permissible number of electrons