

# Structure of Atom

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## Constants and Formulae to Remember

- Avogadro's number  $N_A = 6.022 \times 10^{23}$
- Charge on Electron =  $1.6 \times 10^{-19}$  C
- Mass of Electron =  $9.1 \times 10^{-31}$  kg
- Mass of Proton = Mass of Neutron =  $1.67 \times 10^{-27}$  kg
- Planck's Constant  $h = 6.626 \times 10^{-34}$  J s
- Speed of light  $c = 3 \times 10^8$  m/s
- 1 Electron Volt (eV) =  $1.6 \times 10^{-19}$  J
- Equation of wave motion  $c = \lambda \times \nu$
- Energy of a quantum  $E = h\nu = \frac{hc}{\lambda} = \frac{19.8 \times 10^{-26}}{\lambda} J = \frac{1237}{10^9 \lambda} eV$
- Incident Energy by Light  $E = E_0 + KE$
- Angular momentum of an orbit  $mvr = \frac{nh}{2\pi}$
- Velocity of an electron in Bohr's model =  $2.18 \times 10^8 \frac{Z}{n}$  cm/s =  $2.18 \times 10^6 \frac{Z}{n}$  m/s
- No. of revolutions of an electron in Bohr's model =  $\frac{v}{2\pi r}$
- Radius of an orbit/shell in Bohr's model  $r = r_0 \frac{n^2}{Z}$

where  $r_0 = 0.529 \text{ \AA}$ .

- Energy of an electron in an orbit/shell in Bohr's model  $E = E_0 \frac{Z^2}{n^2}$

where  $E_0 = -2.18 \times 10^{-18}$  J per atom

or  $E_0 = -13.6$  eV per atom

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or  $E_0 = -1312$  kJ per mole

- Potential Energy of an electron  $U = \frac{-kZe^2}{r}$
- Kinetic Energy of an electron  $KE = \frac{kZe^2}{2r}$
- Total Energy of an electron  $TE = \frac{-kZe^2}{2r} = - KE$

- Rydberg Constant =  $109677 \text{ cm}^{-1} = 2.18 \times 10^{-18} \text{ J}$

$$\text{or } \frac{1}{R_H} = 912 \text{ \AA}$$

- If an electron jumps from the  $n_2$  orbit to the  $n_1$  orbit, then its:

$$\text{Wavelength} \Rightarrow \frac{1}{\lambda} = R_H Z^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$\text{where } R_H = 109677 \text{ cm}^{-1} \text{ or } \frac{1}{R_H} = 912 \text{ \AA}$$

$$\text{Energy} \Rightarrow \Delta E = R_H Z^2 \left( \frac{1}{n_{\text{initial}}^2} - \frac{1}{n_{\text{final}}^2} \right)$$

$$\text{where } R_H = 2.18 \times 10^{-18} \text{ J}$$

$$\text{No. of emitted lines} = \frac{(n_2 - n_1)(n_2 - n_1 + 1)}{2}$$

- Ionization Energy of an atom =  $R_H Z^2$
- Wavelength of a particle according to de Broglie equation

$$\lambda = \frac{h}{mv} = \frac{h}{p} = \frac{h}{\sqrt{2mKE}} = \frac{h}{\sqrt{2meV}}$$

- Heisenberg's Uncertainty Principle  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi} \Rightarrow \Delta x \cdot \Delta v \geq \frac{h}{4\pi m}$

where  $\frac{h}{4\pi m} = 5.8 \times 10^{-5} \text{ m}^2/\text{s}$

- Schrödinger's wave equation  $\hat{H}\Psi = E\Psi$

where  $\Psi$  is the amplitude of the electron wave (aka wave function), and  $\hat{H}$  is the Hamiltonian operator.

- The radial probability of finding an electron in a region having volume V is

$$\text{Radial Probability} = \Psi^2 dV = \Psi^2 dx \cdot dy \cdot dz = 4\pi r^2 dr \Psi^2$$

- Quantum Numbers:

Quantum Number	Meaning	Values	Examples
Principal (n)	Shell	1, 2, 3, 4, etc.	K, L, M, N
Azimuthal (ℓ)	Subshell	0 to n - 1	s, p, d, f
Magnetic (m <sub>ℓ</sub> )	Orientation / Orbital	-ℓ to +ℓ	p <sub>x</sub> , p <sub>y</sub> , p <sub>z</sub> , d <sub>xy</sub> , d <sub>yz</sub> , d <sub>zx</sub> , d <sub>x<sup>2</sup>-y<sup>2</sup></sub> , d <sub>z<sup>2</sup></sub>
Spin (m <sub>s</sub> )	Spin	$\frac{1}{2}$ or $-\frac{1}{2}$	↑, ↓

- Orbital angular momentum of an electron =  $\frac{h}{2\pi} \sqrt{l(l+1)} = \hbar \sqrt{l(l+1)}$
- Spin angular momentum of an electron =  $\frac{h}{2\pi} \sqrt{s(s+1)} = \hbar \sqrt{s(s+1)}$
- The number of radial nodes is n - ℓ - 1.
- The number of angular nodes is ℓ.
- The total number of nodes is n - 1.

## Fundamentals

Atomic Number Z = Protons + Electrons

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Mass Number  $A = \text{Protons} + \text{Neutrons}$

## **Iso-what now?**

Isotopes - Same atomic number, different mass numbers.

Isobars - Same mass number, different atomic numbers.

Isotones - Same number of neutrons, different mass numbers.

i.e. Isotones have the same number of neutrons but different numbers of protons.

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As we already know, atoms consist of electrons arranged in shells, such as K, L, M, N, etc.

When an electron jumps from a higher shell to a lower shell, it releases energy. Similarly, to jump from lower shell to higher shell, it absorbs energy.

This *energy* is released and absorbed in the form of light. (Surprising, I know!)

Light (along with all other radiations) is both a wave and a particle. Hence, light is also called *electromagnetic radiation* or *electromagnetic wave*. First, we are going to consider it in the form of a wave. Later, in [Planck's Quantum Theory](#), we are going to consider it as a stream of particles.

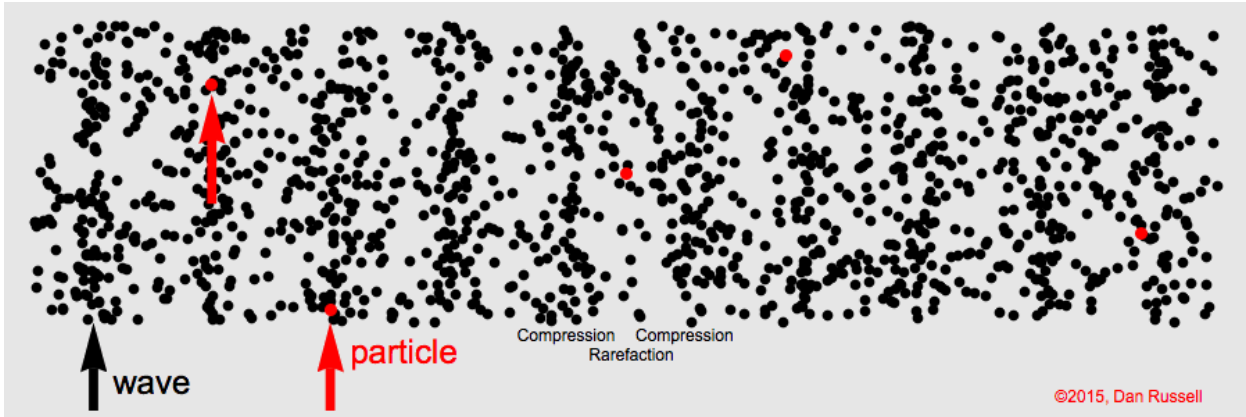
There are some concepts related to waves that will naturally apply to light too, and as a result, they'll also apply to the energy released by atoms.

These concepts are explained below.

## **Wave Motion**

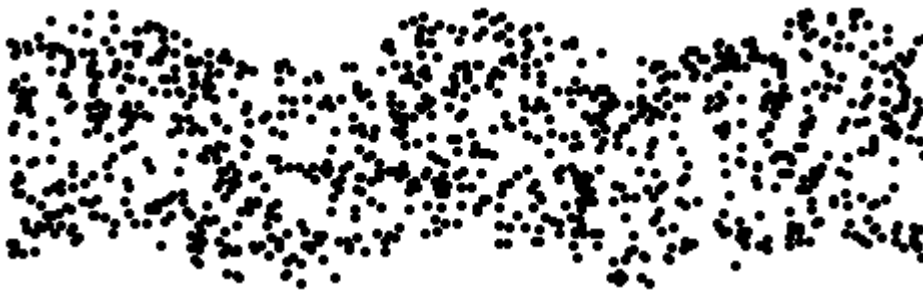
There are two types of waves - Longitudinal Waves, and Transverse Waves.

In a longitudinal wave the particles move parallel (in the same direction) to the direction of the wave, as shown here:



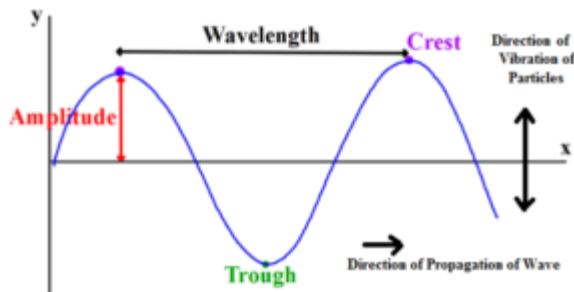
E.g.: Sound waves are longitudinal waves.

In a transverse wave the particles move perpendicular to the direction of the wave, as shown here:



E.g.: Light waves (aka electromagnetic radiations) are transverse waves.

The following diagram shows some of the parts of a wave:



The top-most points are called *crests*, while the bottom-most points are called *troughs*.

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**Wavelength ( $\lambda$ )** - It is the distance between 2 adjacent crests or 2 adjacent troughs. It is denoted by lambda  $\lambda$ .

**Frequency ( $\nu$ )** - It is the number of waves passing through a point in 1 second. It is denoted by nu  $\nu$ . SI Unit of frequency is  $s^{-1}$  or Hertz (Hz).

$$\nu = \frac{1}{T}$$

**Velocity ( $c$ )** - It's the distance travelled by a wave in one second. For light (or electromagnetic radiations), it's the speed of light, obviously.

**Amplitude ( $a$ )** - It is the height of a crest or the depth of a trough.

It tells us the brightness/intensity of light.

**Wave Number ( $\bar{\nu}$ )** - It is the number of wavelengths per metre or centimetre. It is denoted by nu bar  $\bar{\nu}$ .

### Equations of Wave Motion

$$\bar{\nu} = \frac{1}{\text{Wavelength}} = \frac{1}{\lambda}$$

As Speed =  $\frac{\text{Distance}}{\text{Time}}$ ,

$$c = \frac{\lambda}{T}$$

$$[\because \nu = \frac{1}{T}]$$

$$c = \lambda \times \nu$$

$$\Rightarrow \nu = \frac{c}{\lambda}$$

$$[\because \frac{1}{\lambda} = \bar{\nu}]$$

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$$\therefore v = c \times \bar{\nu}$$

$$\text{velocity } v = \lambda \times \nu$$

## Electromagnetic Spectrum

Light (aka electromagnetic radiation) comes in various frequencies, from UltraViolet light to visible light to infrared light and everything else in between.

So, the arrangement of these different types of electromagnetic radiation in the order of increasing wavelengths (or decreasing frequencies) is called the electromagnetic spectrum.

The order of **increasing wavelengths** is:

Gamma rays < X-Rays < UV < Visible Radiations < Infrared < Microwaves < Radio Waves

## Planck's Quantum Theory

Earlier, the electromagnetic wave theory said that the radiant energy is released and absorbed continuously, but this couldn't explain the behaviour of the [photoelectric effect](#).

So, according to Planck's Quantum Theory, the radiant energy from electrons is not emitted or absorbed continuously, but *discontinuously* in the form of small packets called quanta. Each quanta has a fixed amount of energy. In the case of light, the quanta have a special name - photons. Hence here, we're considering light is made up of particles called photons.

The energy of a quantum is given by Planck's equation as

$$E = h\nu$$

where h is the Planck's constant ( $6.626 \times 10^{-34}$  J s)

The energy of a body is an integral multiple of the energy of 1 quantum, so

$$E = nh\nu = \frac{nhc}{\lambda}$$

where n is an integer like 1, 2, 3, etc.

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Planck's equation shows why violet has more energy than red (as energy is directly proportional to frequency).

The energy possessed by 1 mole of quanta is called 1 Einstein of energy.

$$1 \text{ Einstein} = N_A h\nu$$

where  $N_A$  is Avogadro's number ( $6.022 \times 10^{23}$ ).

## **Photoelectric Effect**

The phenomenon in which electrons are instantly emitted from the surface of a photoelectric material when light (photons) falls on it is called the photoelectric effect.

The emitted electrons are called photoelectrons.

The photoelectric effect is used in solar panels to produce electricity from sunlight.

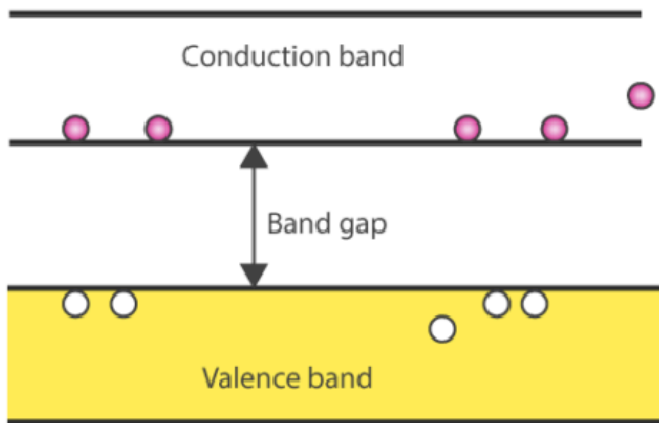
The photoelectric materials are usually metals.

When an electron is energized, it jumps from the ground state to the excited state, as explained below:

Atoms have 2 bands - valence band, and conduction band.

Normally, the outermost electrons of an atom are present in the valence band. When struck by energy from photons, the electrons jump up from the valence band to the conduction band by overcoming the band gap. This movement of electrons produces electric current.





For each metal, a minimum frequency of light is required to eject electrons. This is called threshold frequency ( $\nu_0$ ). Light of frequency less than the threshold frequency simply *cannot* eject electrons, no matter how long it falls on the material.

Hence, the minimum energy required to eject an electron is  $E_0 = h\nu_0$ , and is also called as work function  $w_0$ .

Each photon energizes 1 electron.

When a photon strikes the surface of a metal, some of its energy is used up to eject the electron, and the remaining energy is transferred to the ejected electron as *kinetic energy*.

Energy of striking photon = Threshold Energy + Kinetic energy of ejected electron

$$E = E_0 + KE$$

$$h\nu = h\nu_0 + KE$$

$$\Rightarrow \frac{hc}{\lambda} = \frac{hc}{\lambda_0} + KE$$

As the intensity of light increases, the number of photons striking the surface increases, and therefore the number of ejected electrons also increases. Hence, the photoelectric current is directly proportional to the intensity/brightness of light.

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*Photoelectric current* doesn't depend on the frequency of light. It just needs the frequency of light to be above the threshold frequency of the metal.

However, the excess frequency of light is converted to kinetic energy of the electron. So, *kinetic energy* depends on the frequency of light.

Hence, as frequency of light increases, the kinetic energy increases, and the stopping potential also increases (the electron needs more energy to stop itself after getting ejected). (Stopping potential is just the amount of volts required to stop a moving electron.)

In other words, photoelectric current *only* depends on intensity of light, and kinetic energy *only* depends on frequency of light.

## Bohr's Atomic Model

Bohr's Atomic Model only applies to Hydrogen and Hydrogen-like atoms (i.e. atoms which have only 1 electron).

### Postulates of Bohr's Model

- An atom consists of a small and heavy nucleus in its centre, which is surrounded by electrons.
- The electrons orbit around an atom in circular paths called as *orbits*, *stationary orbits*, or *stationary states*.
- Each orbit has a fixed radius and energy, hence orbits are also called *energy levels* or *energy shells*.
- The orbits are numbered as 1, 2, 3, 4, etc. or named as K, L, M, N, etc.
- The angular momentum of each *orbit* is a whole number multiple of  $\frac{h}{2\pi}$ . Therefore,

$$\text{angular momentum of an orbit } mvr = \frac{nh}{2\pi}$$

where n is the shell number (1, 2, 3, 4, etc.), aka the *principal quantum number*.

- Energy is only absorbed or emitted when electrons jump from one shell to another:
  - When an electron jumps from a lower shell to a higher shell, energy is absorbed.

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- When an electron jumps from a higher shell to a lower shell, energy is released.

Normally, electrons are in their *ground state* and are stable, but when they absorb energy, electrons go into their *excited state* and become unstable.

For Hydrogen and Hydrogen-like atoms, the first shell ( $n = 1$ ) is the ground state. The following shells ( $n = 2, 3, 4$ , etc.) are the first excited state, second excited state, third excited state, and so on.

## Radius of an Orbit

The radius of an orbit of a Hydrogen/Hydrogen-like atom can be found using:

$$r = r_0 \frac{n^2}{Z}$$

where  $Z$  is the atomic number,  $n$  is the shell number, and  $r_0 = 0.529 \text{ \AA}$ .

## Velocity of an Electron in an Orbit

The velocity of an electron in an orbit of a Hydrogen/Hydrogen-like atom is given by:

$$v = 2.18 \times 10^8 \frac{Z}{n} \text{ cm/s}$$

$$v = 2.18 \times 10^6 \frac{Z}{n} \text{ m/s}$$

## No. of Revolutions of an Electron in an Orbit

$$\text{Number of revolutions} = \text{frequency} = \nu = \frac{1}{T} = \frac{1}{\frac{\text{Distance}}{\text{Speed}}} = \frac{\text{Speed}}{\text{Distance}} = \frac{v}{2\pi r}$$

$$\Rightarrow \text{No. of revolutions} = \frac{v}{2\pi r}$$

Here, the velocity and radius can be calculated using the aforementioned formulas.

## Energy of an Electron in an Orbit

The energy of an electron in an orbit of an Hydrogen/Hydrogen-like atom can be found using:

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$$E = E_0 \frac{Z^2}{n^2}$$

where  $E_0 = -2.18 \times 10^{-18}$  J per atom

or  $E_0 = -13.6$  eV per atom

or  $E_0 = -1312$  kJ per mole

The energy of an electron in an atom is negative because it's considered relative to the energy of a *free electron*, and the energy of a free electron is 0.

### Potential Energy

Potential Energy of an electron  $PE = \frac{-kZe^2}{r}$

### Kinetic Energy

Kinetic Energy of an electron  $KE = \frac{kZe^2}{2r}$

### Total Energy

Total Energy of an electron  $TE = PE + KE = \frac{-kZe^2}{2r} = - KE$

## Atomic Spectrum

When sunlight is passed through a prism, it forms a *continuous spectrum* of all visible colours.

We know that electrons emit and absorb energy in the form of light. However, when *that* light is passed through a prism, it forms a spectrum which is **not** continuous. It consists of lines or bands of fixed frequencies, and is called *discontinuous spectrum*, *line spectrum*, or *atomic spectrum*. It is different for different elements, and is hence called the "fingerprint" of an element.

The atomic spectrum is of 2 types:

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1. Emission Spectrum
  2. Absorption Spectrum

**Emission Spectrum:** When an electron has absorbed energy, it **emits** it in the form of radiation which makes a spectrum with *coloured* lines/bands.

**Absorption Spectrum:** When light is passed through an electron and later observed, it makes a spectrum with *dark* lines/bands.

The dark bands in the absorption spectrum are in the exact same places as the coloured bands in the emission spectrum.

### Hydrogen Spectrum

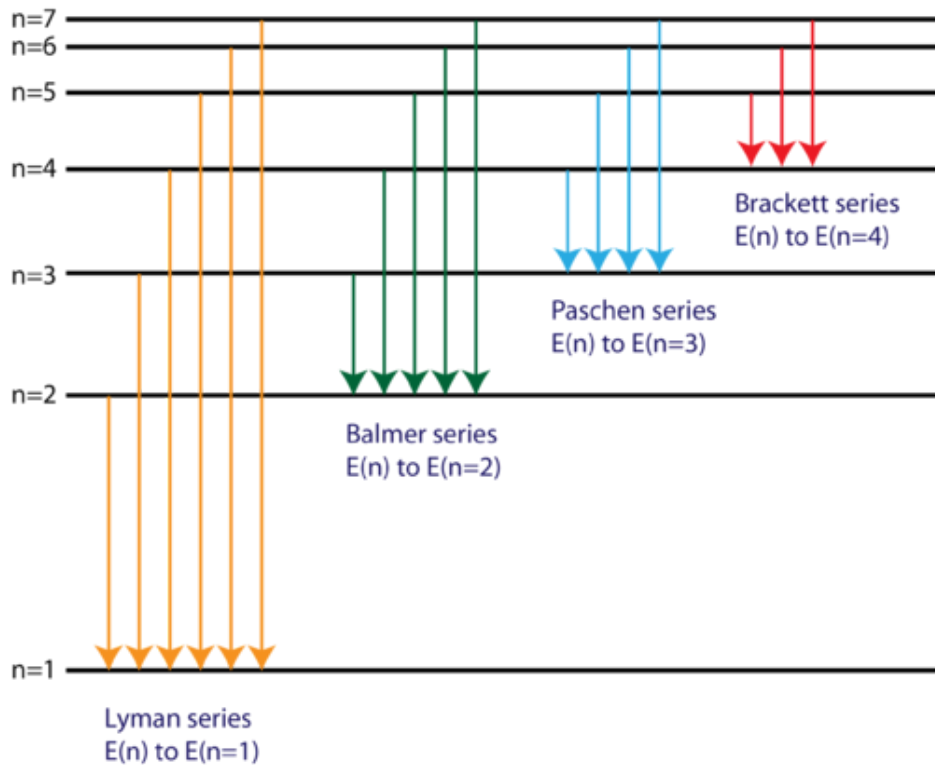
The Hydrogen Spectrum is also called the Hydrogen Line Spectrum.

It consists of *lots* of lines in various regions, which are grouped into the following series:

**Lyman < Balmer < Paschen < Brackett < Pfund < Humphrey**

The Lyman series is present in the UV region, the Balmer series is in the visible region, and the rest are in the Infrared region.

The first 4 series are shown below:



- When an electron jumps from any shell to the first shell ( $n = 1$ ), it is in the Lyman series.
- When an electron jumps from any shell to the second shell ( $n = 2$ ), it is in the Balmer series.
- When an electron jumps from any shell to the third shell ( $n = 3$ ), it is in the Paschen series.
- When an electron jumps from any shell to the fourth shell ( $n = 4$ ), it is in the Brackett series.
- When an electron jumps from any shell to the fifth shell ( $n = 5$ ), it is in the Pfund series.
- When an electron jumps from any shell to the sixth shell ( $n = 6$ ), it is in the Humphrey series.

The maximum amount of energy is released when the line is the longest, i.e, when the electron jumps from infinity to a particular shell. As  $E \propto \frac{1}{\lambda}$ , the shortest wavelength will be present in this case. This longest line with the **shortest wavelength** is called the *limiting line*.

If the electron jumps only one shell, then the wavelength will be the longest in that case.

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## Rydberg Equation

If an electron jumps from the  $n_2$  orbit to the  $n_1$  orbit, then its wavelength can be calculated using the Rydberg equation:

$$\frac{1}{\lambda} = R_H Z^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

where  $R_H = 109677 \text{ cm}^{-1}$

$$\text{or } \frac{1}{R_H} = 912 \text{ \AA}$$

$R_H$  is a form of the Rydberg constant.

Here,  $n_1 < n_2$  so that  $\lambda$  can be positive.

If an electron jumps from the orbit with  $E_{\text{initial}}$  energy to the orbit with  $E_{\text{final}}$  energy, then the energy absorbed or emitted by the electron is

$$\Delta E = E_{\text{final}} - E_{\text{initial}} = R_H Z^2 \left( \frac{1}{n_{\text{initial}}^2} - \frac{1}{n_{\text{final}}^2} \right)$$

where  $R_H = 2.18 \times 10^{-18} \text{ J}$

Here  $R_H$  is called the Rydberg unit of energy (just another form of the Rydberg constant).

**If the energy is negative, then it is emitted. If the energy is positive, then it is absorbed.**

The frequency and wavelength of the absorbed or emitted electron can then also be found using the previously known formula:

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

$$\Rightarrow \nu = \frac{E_f - E_i}{h} \text{ and } \lambda = \frac{hc}{E_f - E_i}$$

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While calculating the frequency and wavelength, the negative sign of energy can be ignored.

### Ionization Energy

The *ionization energy* is the amount of energy required to remove an electron **completely** from an atom (i.e., the electron jumps from  $n=1$  to  $n=\infty$ ).

Ionization Energy =

$$\Delta E = E_{final} - E_{initial} = E_{\infty} - E_1 = R_H Z^2 \left( \frac{1}{n_{initial}^2} - \frac{1}{n_{final}^2} \right) = R_H Z^2 \left( \frac{1}{1^2} - \frac{1}{\infty^2} \right) = R_H Z^2$$

where  $R_H = 2.18 \times 10^{-18} \text{ J}$

Therefore,  $R_H Z^2$  is the ionization energy or *ground state energy* of Hydrogen/Hydrogen-like elements.

The first excitation energy is  $\Delta E = E_{final} - E_{initial} = E_2 - E_1$

The second excitation energy is  $\Delta E = E_{final} - E_{initial} = E_3 - E_2$ , and so on.

### No. of Spectral Lines

The number of lines emitted in the Hydrogen spectrum when an electron jumps from  $n_2$  shell to  $n_1$  shell is  $\frac{(n_2 - n_1)(n_2 - n_1 + 1)}{2}$

### Demerits of Bohr's Atomic Model

Bohr's Atomic Model only worked for Hydrogen and Hydrogen-like atoms.

It couldn't explain the splitting of spectral lines in the presence of magnetic field (*Zeeman effect*) and electric field (*Stark effect*) in the line spectrum of Hydrogen or Hydrogen-like atoms.

Also, it couldn't explain the dual nature of matter as both waves and particles, and only considered matter to be particles.



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## Dual Nature of Matter

Einstein and de Broglie suggested that matter is *both* a wave and a particle.

### de Broglie's Equation

As  $E = mc^2$  and  $E = \frac{hc}{\lambda}$ ,

$$mc^2 = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{h}{mc} = \frac{h}{mv}$$

Therefore, the wavelength of a particle is given by de Broglie's equation as

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

Where  $m$  is the mass,  $v$  is the velocity and  $p$  is the momentum of the particle.

This equation shows that the wavelength of a particle is inversely proportional to its momentum.

The waves are called *matter waves* or *de Broglie waves*. **The number of these waves in the  $n^{\text{th}}$  orbit is  $n$ .**

### Relationship between Kinetic Energy and Wavelength

$$\text{Kinetic Energy } KE = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{(mv)^2}{m} = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mKE}$$

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

### Relationship between Kinetic Energy and Potential Difference

1 eV is the amount of **kinetic energy** gained/lost by an electron, which is accelerated from rest, through an **electric potential difference of 1 Volt**.

If  $e$  is the charge of an electron,

$$1 \text{ eV} = e \times V = 1.6 \times 10^{-19} \text{ C} \times 1 \text{ V} = 1.6 \times 10^{-19} \text{ J}$$

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Since kinetic energy is also equal to  $\frac{1}{2}mv^2$ ,

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

$$\lambda = \frac{h}{\sqrt{2mKE}} = \frac{h}{\sqrt{2meV}} = \frac{1.226 \times 10^{-9}}{\sqrt{V}} \text{ metres}$$

where V is the potential difference.

## Heisenberg's Uncertainty Principle

According to Heisenberg's Uncertainty Principle, the position and momentum of an electron can't *both* be known accurately at the same time.

That is, if the position is measured accurately, then momentum would be less accurate, and if momentum is measured accurately, then the position would be less accurate.

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

where  $\frac{h}{4\pi m} = 5.8 \times 10^{-5} \text{ m}^2/\text{s}$

## Quantum Mechanical Model of Atom

The quantum mechanical model of atoms was based on the dual nature of matter and Heisenberg's Uncertainty Principle.

## Schrödinger's Wave Equation

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{\delta^2\Psi}{\delta y^2} + \frac{\delta^2\Psi}{\delta z^2} + \frac{8\pi^2 m}{h^2} (E - V)\Psi = 0$$

It can also be written as:

$$\widehat{H}\Psi = E\Psi$$

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where  $\Psi$  (psi) is the *amplitude of the electron wave* (aka *wave function*), and  $\hat{H}$  is the *Hamiltonian operator*.

### Significance of $\Psi$ and $\Psi^2$

$\Psi$  (psi) is the *amplitude* of the wave of an electron, and is also called a *wave function*.

The amplitude of the electron wave, or wave function ( $\Psi$ ) can be expressed in terms of Cartesian coordinates (x, y, z) or spherical polar coordinates (r,  $\Theta$ ,  $\Phi$ ).

When Schrödinger's wave equation is solved, it gives many values of  $\Psi$ . The real values of  $\Psi$  are called *eigenvalues* and the corresponding wave functions ( $\Psi$ ) are called *eigenfunctions*.

Since the square of amplitude gives us the intensity of radiation,  $\Psi^2$  tells us the intensity of an electron, i.e., the probability of finding the electron at a particular point in an atom.

Hence,  $\Psi$  is called the *probability amplitude* and  $\Psi^2$  is called the *probability density* of an electron's wave.

$\Psi$  may be positive or negative depending on the values of the coordinates, but  $\Psi^2$  is always positive.

In Bohr's atomic model, each atom has separate orbits in which electrons could *definitely* be found.

But in the quantum mechanical model, it has been replaced by the probability density ( $\Psi^2$ ), where electrons *may or may not* be found.

A high  $\Psi^2$  means electrons are more likely to be found at that point, and a low  $\Psi^2$  means electrons are less likely to be found there. If  $\Psi^2$  is 0, it means electrons can't be found there.

The most probable regions in which electrons are highly likely to be found are called *atomic orbitals* (s, p, d, f).

Hence, orbitals are defined as the region around the nucleus where the probability of finding an electron is maximum.

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The places where the probability density is zero are called *nodes*.

## Quantum Numbers

The solution of Schrödinger's wave equation gives 3 quantum numbers -  $n$ ,  $l$ , and  $m_l$ . A fourth quantum number ( $m_s$ ) was later created to describe an electron's spin.

Together, these 4 quantum numbers can completely describe an electron in an atom.

1. Principal Quantum Number ( $n$ )
2. Azimuthal Quantum Number ( $l$ )
3. Magnetic Quantum Number ( $m_l$ )
4. Spin Quantum Number ( $m_s$ )

### Principal Quantum Number ( $n$ )

It is the **shell** of the electron.

It has values  $n = 1, 2, 3, 4$ , etc. or also written as  $n = K, L, M, N$ , etc.

It can be used to know the:

- distance of the electron from the nucleus (using [this formula](#))
- energy of the electron (using [this formula](#))

The maximum number of *electrons in each shell* is  $2n^2$ .

### Azimuthal Quantum Number ( $l$ )

It is the **subshell** of the shell.

It has values from  $l = 0$  to  $n - 1$  (s, p, d, f, etc.)

The number of *subshells in each shell* is  $n$ .

It can be used to know the:

- number of subshells in a shell

- relative energies of the subshells ( $s < p < d < f$ ) (except in Hydrogen, where the subshells of a particular shell have the same energy)
- orbital angular momentum of an electron

The azimuthal quantum number is also called the *angular* quantum number.

### Orbital Angular Momentum

$$\text{Orbital angular momentum of an electron} = \frac{h}{2\pi} \sqrt{l(l+1)} = \hbar \sqrt{l(l+1)}$$

where  $\hbar$  is a shortcut way of writing  $\frac{h}{2\pi}$  and is called the *reduced Planck's constant*.

Note - The angular momentum of an *orbit* is  $\frac{nh}{2\pi}$ , but the above is the angular momentum of an *orbital*.

### Magnetic Quantum Number ( $m_\ell$ )

It is the **orientation** of the subshell. The subshell with a specific orientation is called an orbital.

It has values from  $m_\ell = -\ell$  to  $+\ell$ .

- The s subshell has 1 orbital, called the s-orbital.
- The p subshell has 3 orbitals, called  $p_x$ ,  $p_y$ , and  $p_z$  orbitals.
- The d subshell has 5 orbitals, called  $d_{xy}$ ,  $d_{yz}$ ,  $d_{zx}$ ,  $d_{x^2-y^2}$ , and  $d_{z^2}$  orbitals.

The number of orbitals in each subshell is  $2\ell + 1$ .

### Spin Quantum Number ( $m_s$ )

It is the **spin orientation** of the electron. It can be clockwise or anticlockwise.

It has values  $\frac{1}{2}$  or  $-\frac{1}{2}$  and is also shown using arrows  $\uparrow$  or  $\downarrow$ .

### Spin Angular Momentum

Apart from angular momentum of an *orbit* and angular momentum of an *orbital*, there's also angular momentum of the *spin* of an electron.

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$$\text{Spin angular momentum of an electron} = \frac{h}{2\pi} \sqrt{s(s+1)} = \hbar \sqrt{s(s+1)}$$

where  $\hbar$  is a shortcut way of writing  $\frac{h}{2\pi}$  and is called the *reduced Planck's constant*.

So, in summary:

Quantum Number	Meaning	Values	Examples
Principal (n)	Shell	1, 2, 3, 4, etc.	K, L, M, N
Azimuthal (ℓ)	Subshell	0 to n - 1	s, p, d, f
Magnetic (m <sub>ℓ</sub> )	Orientation / Orbital	-ℓ to +ℓ	p <sub>x</sub> , p <sub>y</sub> , p <sub>z</sub> , d <sub>xy</sub> , d <sub>yz</sub> , d <sub>zx</sub> , d <sub>x<sup>2</sup>-y<sup>2</sup></sub> , d <sub>z<sup>2</sup></sub>
Spin (m <sub>s</sub> )	Spin	1/2 or -1/2	↑, ↓

## Shapes of Orbitals

The shapes of orbitals are obtained from the graphs of  $\Psi$  and  $\Psi^2$ .

When the wave function  $\Psi$  is expressed as a function of radius r (distance from the nucleus), it is called a *radial wave function*.

It can be shown by the graph of  $\Psi$  with r.

The points at which the graph of radial wave function becomes 0 are called *radial nodes*. The probability of finding an electron at that point is zero.

Similarly, when the probability density  $\Psi^2$  is expressed as a function of radius r (distance from the nucleus), it is called a *probability density function*.

The graph of  $\Psi^2$  with r is called *probability density graph*, and gives the probability density of finding an electron at a point.

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The points at which the probability density graph becomes 0 are called *angular nodes* or *nodal planes*.

However, the *total* probability of finding an electron in a region at a distance  $r$  from the nucleus is called *radial probability*.

The radial probability of finding an electron in a region having volume  $V$  is

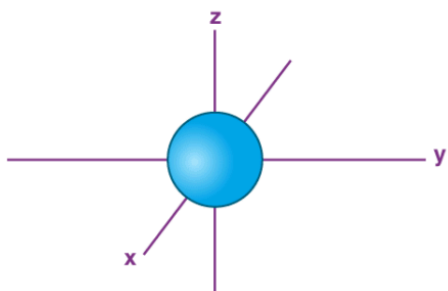
$$\text{Radial Probability} = \Psi^2 dV = \Psi^2 dx \cdot dy \cdot dz = 4\pi r^2 dr \Psi^2$$

The graph of radial probability, i.e., probability expressed as a function of  $r$ , is called the *radial probability distribution function graph*.

The peak of the graph gives the distance from the nucleus where the probability of finding an electron is maximum. It is called the *radius of maximum probability*.

### Shape of s-orbitals

s-orbitals are spherical in shape.

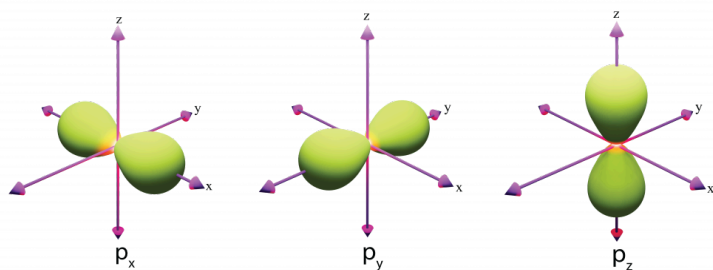


### Shape of p-orbitals

p-orbitals are dumbbell shaped.

They are  $p_x$ ,  $p_y$ , and  $p_z$ .

The 2 lobes of the p-orbital lie on the axis in their names, and are separated by a nodal plane.



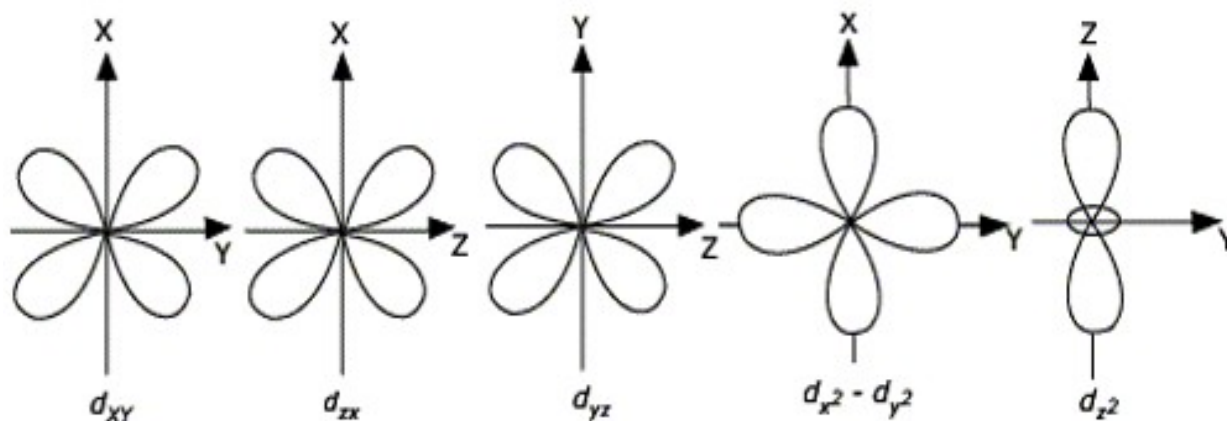
## Shape of d-orbitals

The d-orbitals are  $d_{xy}$ ,  $d_{yz}$ ,  $d_{zx}$ ,  $d_{x^2-y^2}$ , and  $d_{z^2}$ .

The lobes lie in between the axes in the names. For example, in  $d_{xy}$ , the lobes lie in between the x and y axes.

The  $d_{x^2-y^2}$  orbital is just like the  $d_{xy}$  orbital, but rotated  $45^\circ$  around the z-axis.

The  $d_{z^2}$  orbital has a ring of high electron density in the xy plane with 2 lobes in the z-axis.



## Nodes

A *spherical surface* inside an orbital in which the probability of finding an electron is zero is called a **spherical node** or **radial node**. The graph of radial wave function is zero there.

The number of radial nodes is  $n - \ell - 1$ .



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A *plane* passing through the nucleus where the probability of finding an electron is zero is called an **angular node** or **nodal plane**. The graph of the probability density function is zero there.

The number of angular nodes is  $\ell$ .

The total number of nodes is  $n - 1$ .

The number of nodes can also be found by the number of times the graph touches zero.

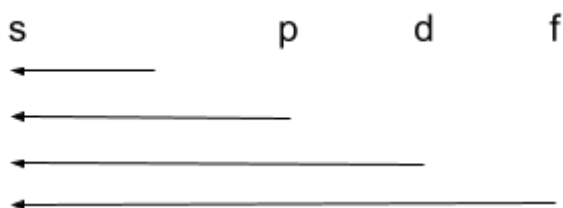
## Signs of Orbitals

The signs on the lobes of orbitals only show the signs of the wave function in that direction.

- The s-orbitals are always positive.
- The opposite lobes of p-orbitals have opposite signs.
- The opposite lobes of d-orbital have the same sign.

## Energies of Orbitals

How to write the increasing energy levels of orbitals:



1. Write the letters of each arrow from the reverse, twice.
2. In other words, first write s s, then p s p s, then d p s d p s, and finally f d p s f d p s.
3. Number each s-orbital from 1, each p-orbital from 2, each d-orbital from 3 and each f-orbital from 4.

The final result is as follows:

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d 7p 8s

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For the same value of  $n$ , the subshell with the higher value of  $\ell$  has more energy.

Energies of orbitals in the same subshell decrease with increase in atomic number. For example, the 2s orbital of sodium has less energy than the 2s orbital of potassium, and so on.

The above applies to multielectron atoms. In Hydrogen atoms, the subshells of the same shell have the same energy. For example, 2s and 2p have the same energy, and 3s, 3p and 3d have the same energy.

This is because there is only one electron in an Hydrogen atom, so there's no screening/shielding effect.

Shielding effect is when the electrons of inner shells *shield* the outermost electrons from the effects of the nucleus, i.e., the effective nuclear charge experienced by the orbital decreases with increase in azimuthal quantum number  $\ell$ , and this decrease in attraction by the nucleus leads to increase in energy of the orbital.

The orbitals having the same energy are called *degenerate orbitals*.

## Electronic Configuration of Atoms

The electronic configuration of atoms is done according to the following rules:

1. Aufbau Principle
2. Bohr-Bury's Rule ( $n + \ell$  Rule )
3. Pauli's Exclusion Principle
4. Hund's Rule of Maximum Multiplicity

### Aufbau Principle

The orbitals are filled in the order of their increasing energies.

'Aufbau' is a German word which means 'building up'.

### Bohr-Bury's Rule ( $n + \ell$ Rule )

Orbitals are filled in the order of increasing values of  $n + \ell$ .

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If the values of  $n + \ell$  are same for 2 orbitals, then the one with lower  $n$  is filled first.

### **Pauli's Exclusion Principle**

An orbital can have a maximum of 2 electrons, and they must have opposite spins.

### **Hund's Rule of Maximum Multiplicity**

Electron pairing won't take place until each orbital has a single electron first.

### **Electronic Configuration of Ions**

When adding or removing electrons from ions, add/remove the electrons from the orbital with the highest value of  $n$  first.

If two orbitals have the same highest value of  $n$ , then add/remove the electron from the orbital with the higher value of  $\ell$ .