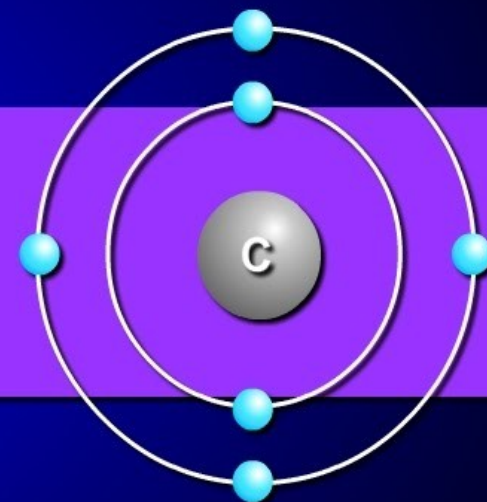




## 2. STRUCTURE OF ATOM

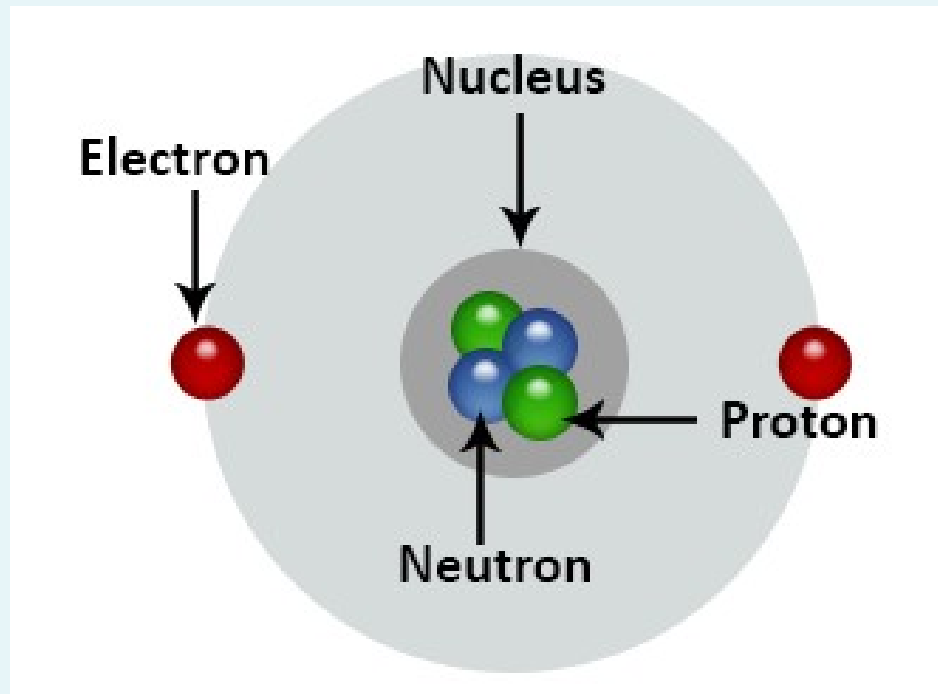


**HAIZEL G.ROY**  
**H.S.S.T. (HG) CHEMISTRY**  
**GOVT. H.S.S. KALAMASSERY**  
**ERNAKULAM**

# **INTRODUCTION**

- According to Dalton's atomic theory, all matter is composed of extremely small particles called atoms.
- The atom consists of smaller particles such as electron, proton and neutron.
- These particles are regarded as fundamental particles.

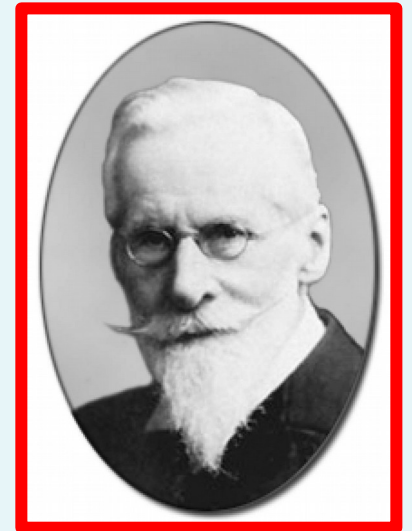
# STRUCTURE OF ATOM



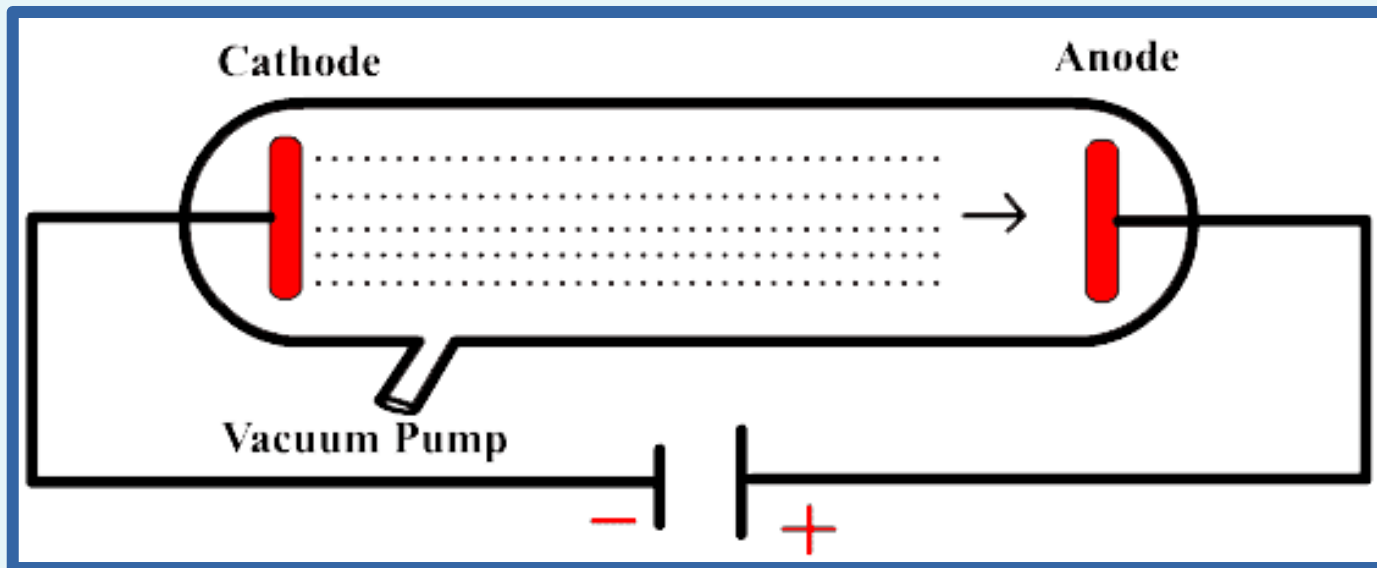
# DISCOVERY OF ELECTRON

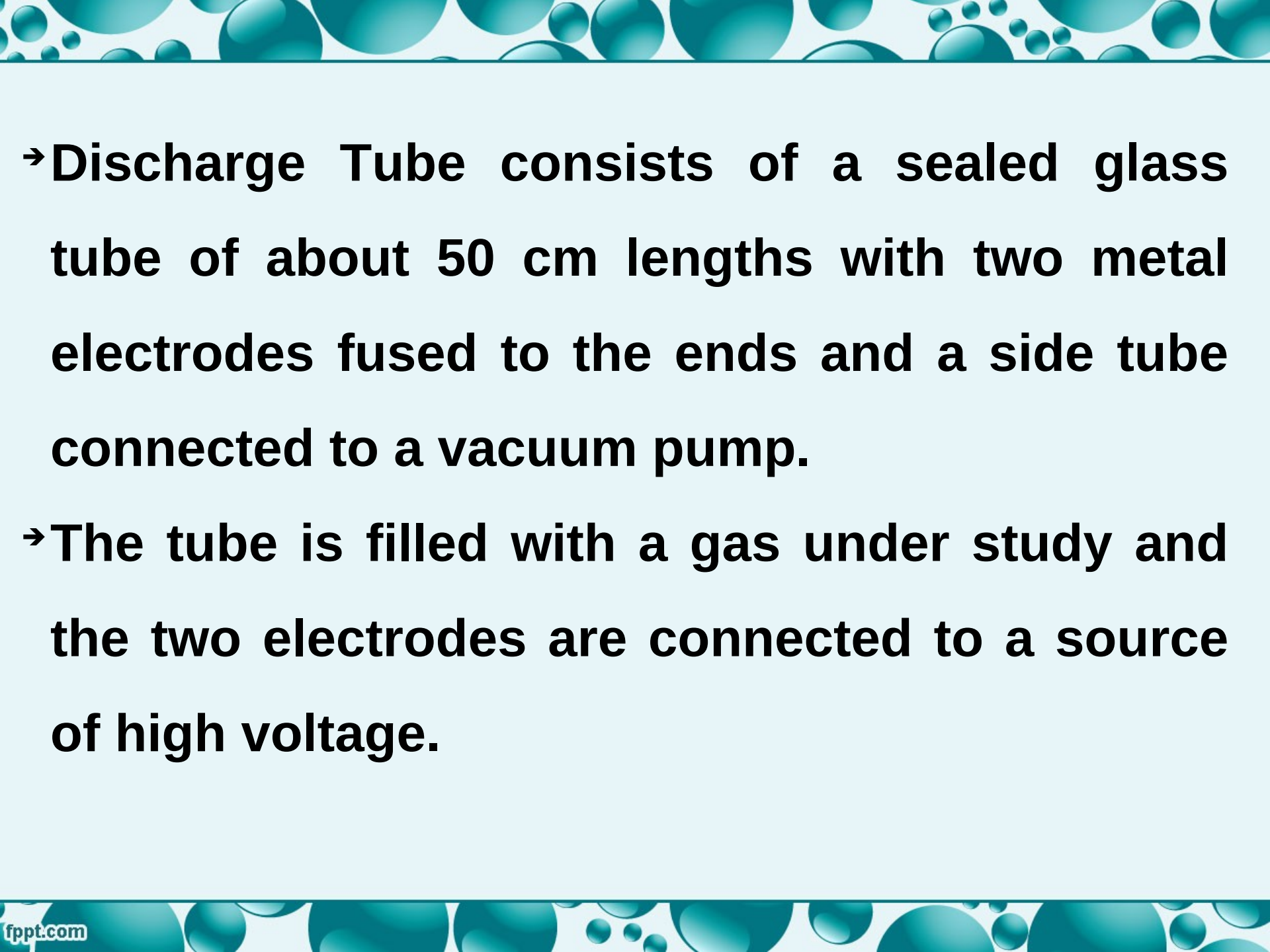
The electrons were discovered by conducting an experiment by using a simple apparatus known as discharge tube or Crookes tube.

**WILLIAM CROOKES**



# DISCHARGE TUBE EXPERIMENT



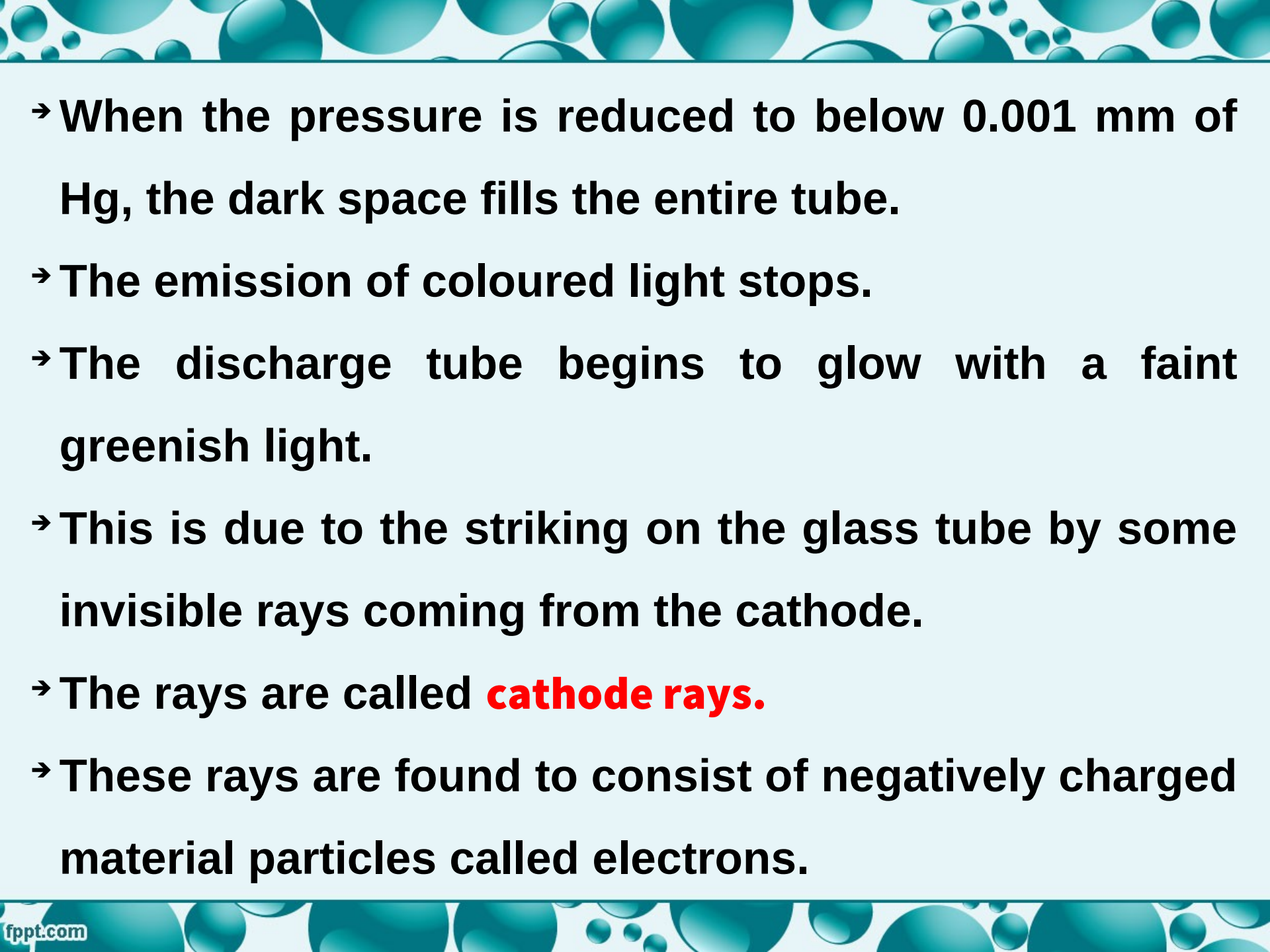
- 
- **Discharge Tube consists of a sealed glass tube of about 50 cm lengths with two metal electrodes fused to the ends and a side tube connected to a vacuum pump.**
  - **The tube is filled with a gas under study and the two electrodes are connected to a source of high voltage.**

# **OBSERVATIONS**

- When the discharge tube containing the gas is at 1 atm pressure and at high voltage, the gas remains non conducting.
- When the pressure of the gas is reduced to about  $10^{-2}$  atm, the gas becomes conducting and light is emitted by the residual gas in the tube.
- The colour of the light depends up on the nature of the gas.

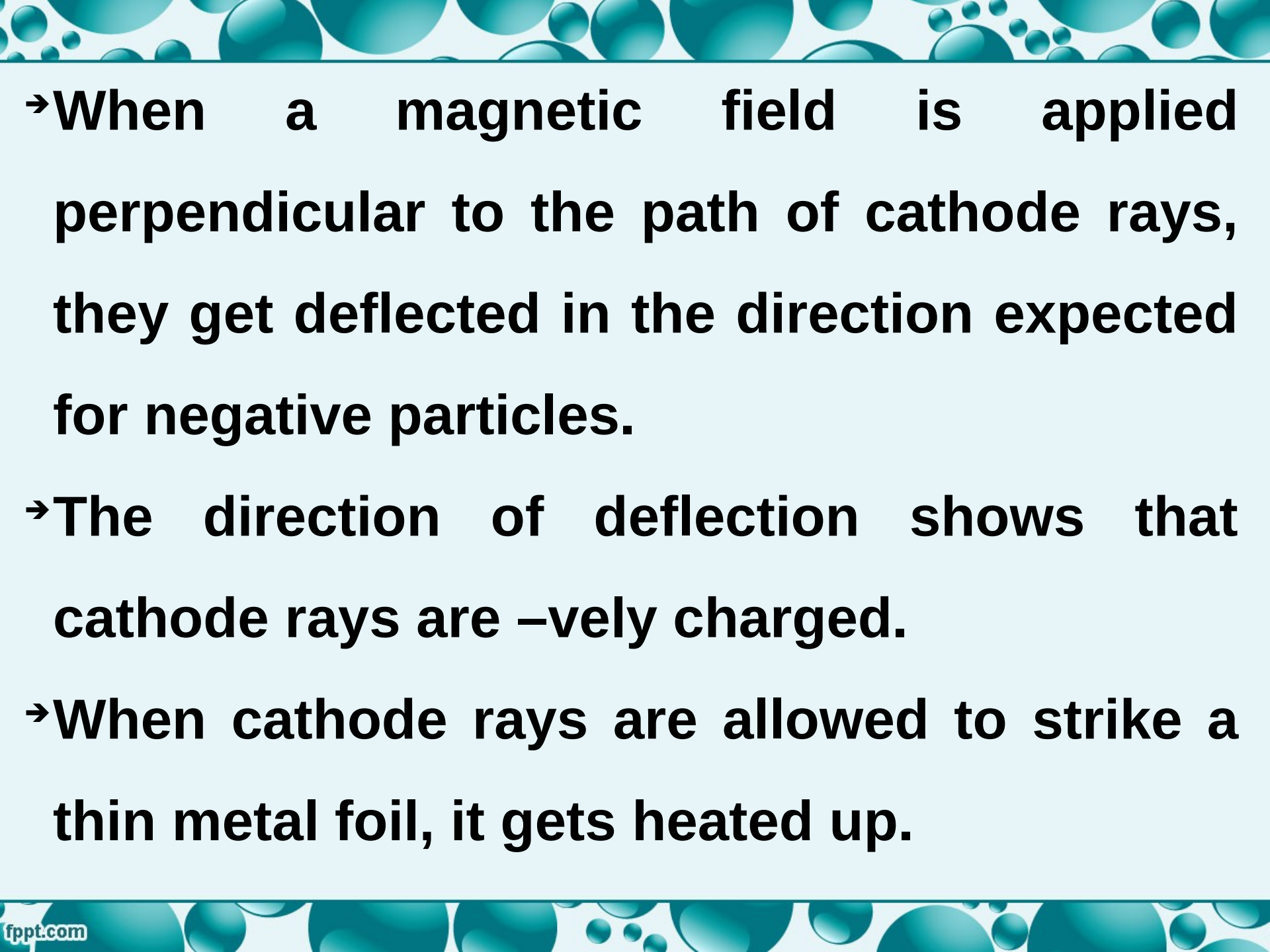
- When the pressure of the gas in the discharge tube is further reduced, the glow becomes weak.
- At about  $10^{-4}$  atm pressure, the glow within the tube stops but the gas continues to conduct electricity.
- The glow surrounding the cathode or the negative electrode detaches itself leaving a space between it and the electrode.
- This is known as **Crookes dark space.**




- 
- When the pressure is reduced to below 0.001 mm of Hg, the dark space fills the entire tube.
  - The emission of coloured light stops.
  - The discharge tube begins to glow with a faint greenish light.
  - This is due to the striking on the glass tube by some invisible rays coming from the cathode.
  - The rays are called **cathode rays**.
  - These rays are found to consist of negatively charged material particles called electrons.

# PROPERTIES OF CATHODE RAYS

- Travel in straight lines.
- Produce mechanical effects.
- When an electric field is applied to a stream of cathode rays, they get deflected towards the positive plate which indicates that cathode rays themselves are **negatively charged.**

- 
- When a magnetic field is applied perpendicular to the path of cathode rays, they get deflected in the direction expected for negative particles.
  - The direction of deflection shows that cathode rays are negatively charged.
  - When cathode rays are allowed to strike a thin metal foil, it gets heated up.

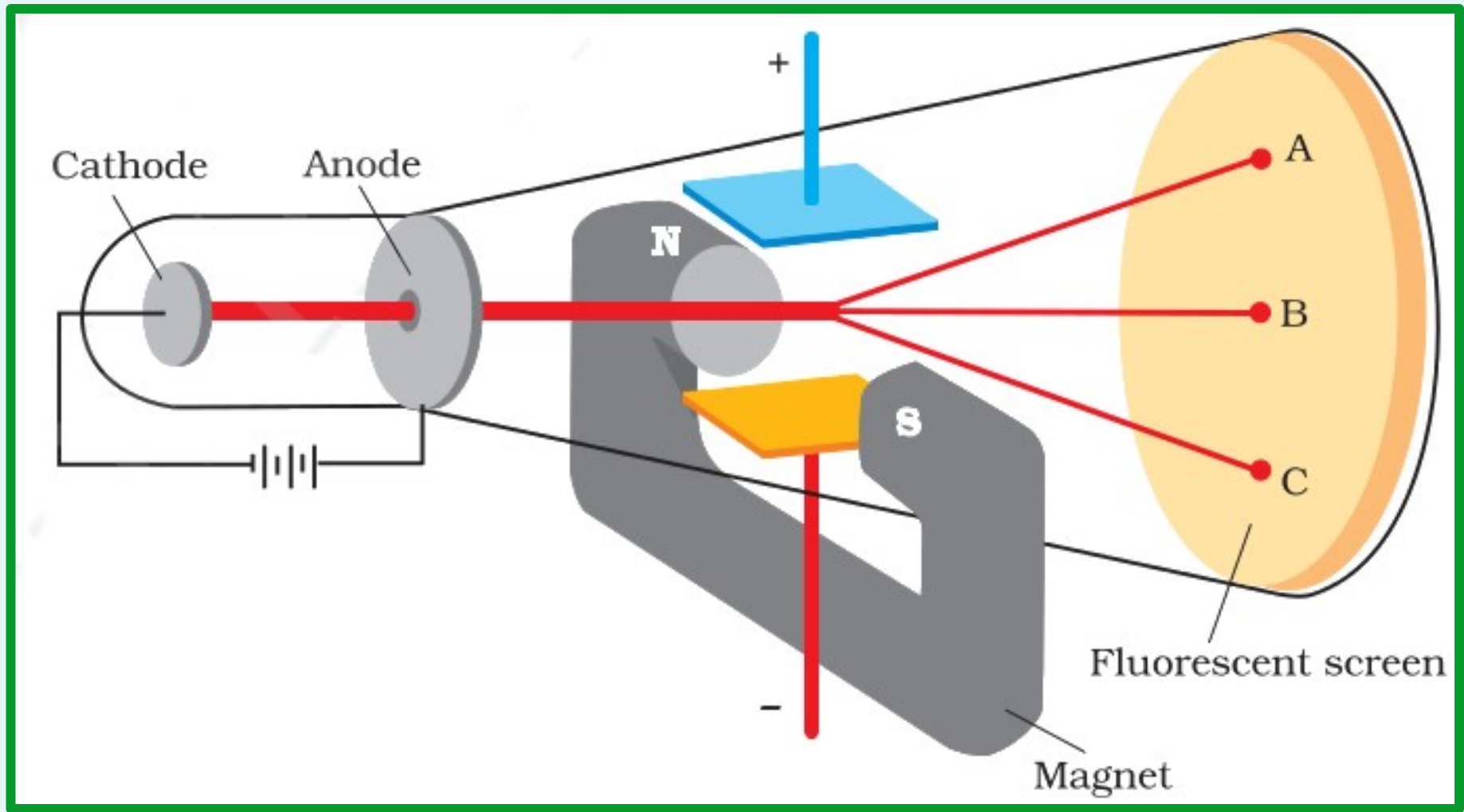
- 
- Produce, x-rays when they strike hard metals like tungsten, copper etc.**
  - Produce fluorescence on glass walls, ZnS etc.**
  - Penetrate through thin metallic foils.**
  - Affect photographic plates.**

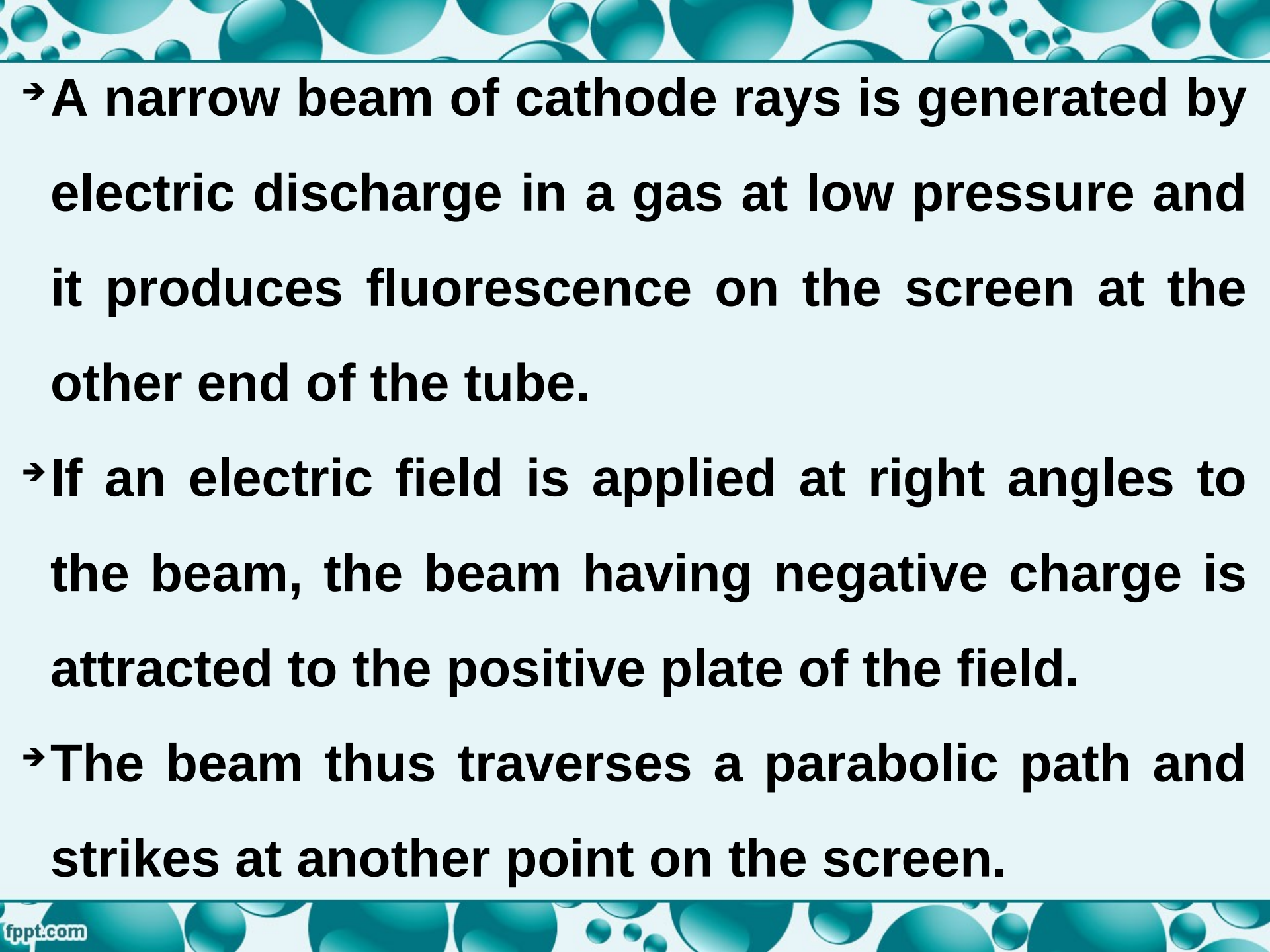
# **DETERMINATION OF CHARGE TO MASS RATIO ( $e/m$ ) OF ELECTRONS**

In 1897 J.J. Thomson determined the  $e/m$  of the electron by measuring the deflection of cathode rays under the simultaneous influence of electric and magnetic fields.

**J.J. THOMSON**





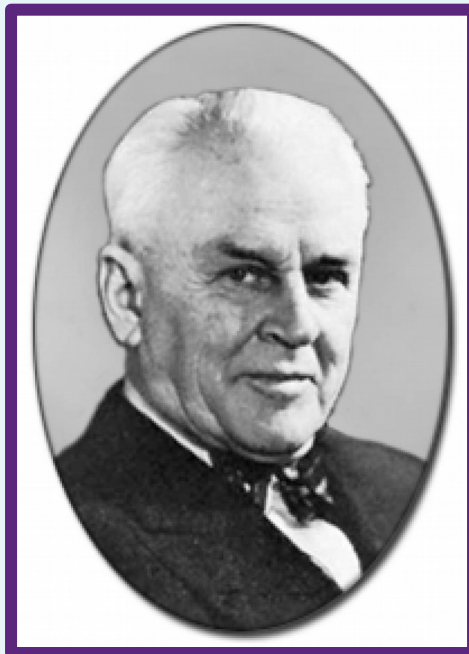
- 
- A narrow beam of cathode rays is generated by electric discharge in a gas at low pressure and it produces fluorescence on the screen at the other end of the tube.
  - If an electric field is applied at right angles to the beam, the beam having negative charge is attracted to the positive plate of the field.
  - The beam thus traverses a parabolic path and strikes at another point on the screen.

- A magnetic field is now applied to the beam in a direction at right angles to that of the electric field.
- The beam undergoes deflection in the opposite direction.
- The strength of the two fields are so adjusted that the beam strikes the screen at the original position.
- From the strength of the two fields, the ratio  $e/m$  can be calculated.
- The  $e/m$  value is found to be  $1.76 \times 10^8$  Coulombs/g.



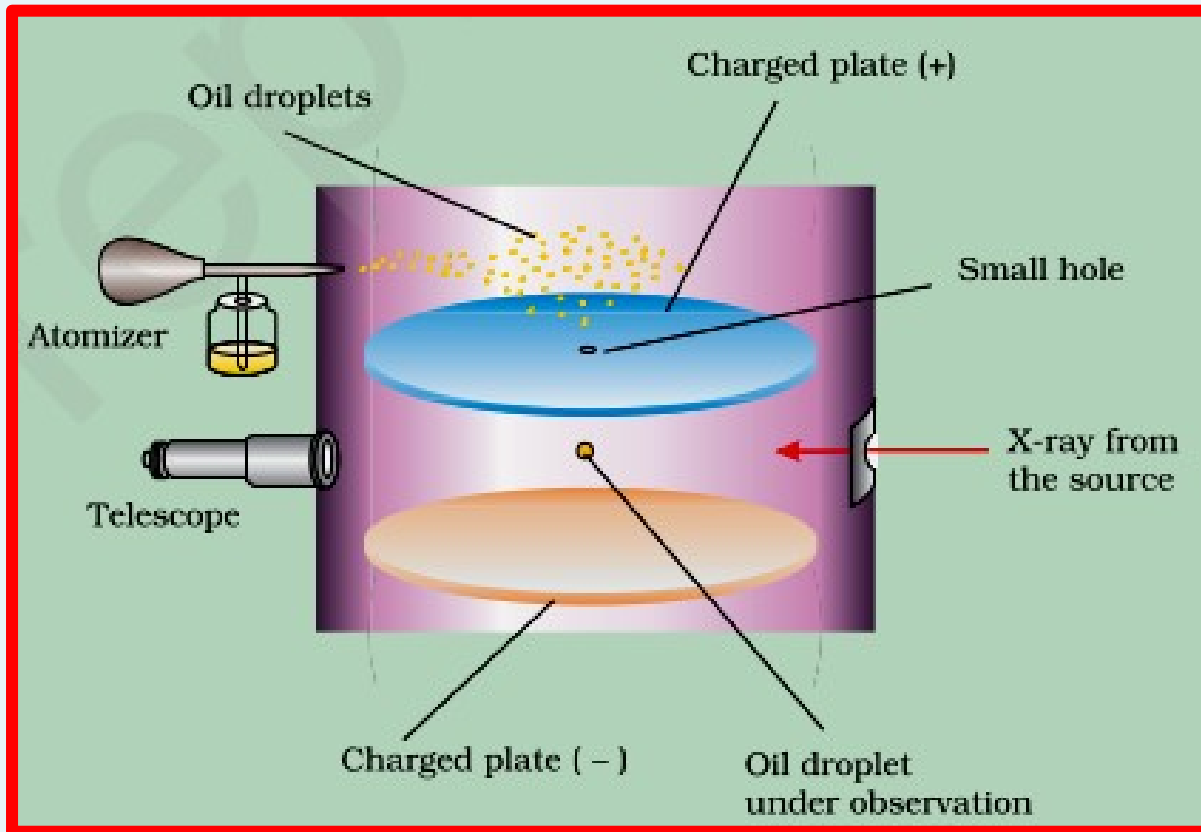
# **DETERMINATION OF CHARGE OF AN ELECTRON**


The charge of an electron was determined by Robert Millikan in 1909 by oil drop experiment.



**ROBERT MILLIKAN**

# MILLIKAN'S OIL DROP EXPERIMENT



- 
- A spray of oil droplets is produced by an atomizer.
  - The oil droplets enter the apparatus through a small hole.
  - It is allowed to fall in between two charged plates.
  - The motion of the droplets is observed with a telescope.
  - The space between the charged plates is irradiated with x-rays.
  - The x-rays ionize the molecules of the air.

- One or more electrons produced may be absorbed by an oil droplet.
- The oil droplet as a result becomes negatively charged.
- By measuring the velocity of a given oil droplet as it falls freely under the influence of gravity and then in an electric field, it is possible to calculate the charge on the droplet which was considered to be electronic charge.
- The charge on the electron is found to be  $1.602 \times 10^{-19}$  coulombs.

# MASS OF AN ELECTRON

From the values of  $e$  and  $e/m$ , the mass ( $m$ ) of the electron is calculated by dividing  $e$  by  $e/m$ .

$$e = 1.602 \times 10^{-19}$$

$$\frac{e}{m} = 1.76 \times 10^8 \text{ C / g}$$

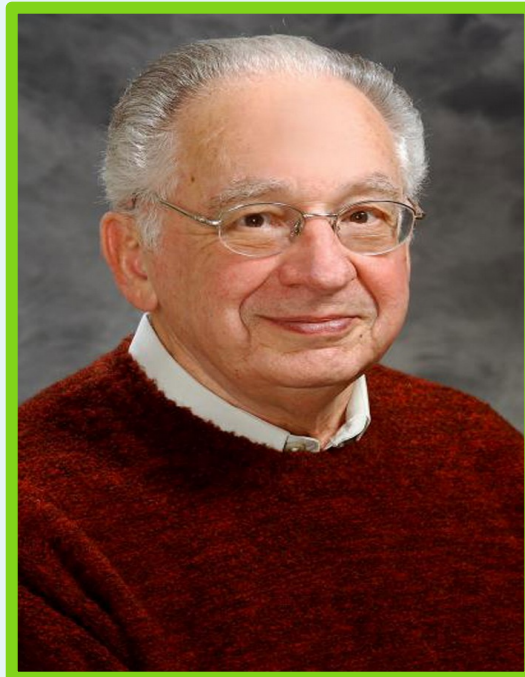
$$\frac{e}{\frac{e}{m}} = \frac{1.602 \times 10^{-19}}{1.76 \times 10^8 \text{ C / g}}$$

$$m = 9.1 \times 10^{-28} \text{ g}$$

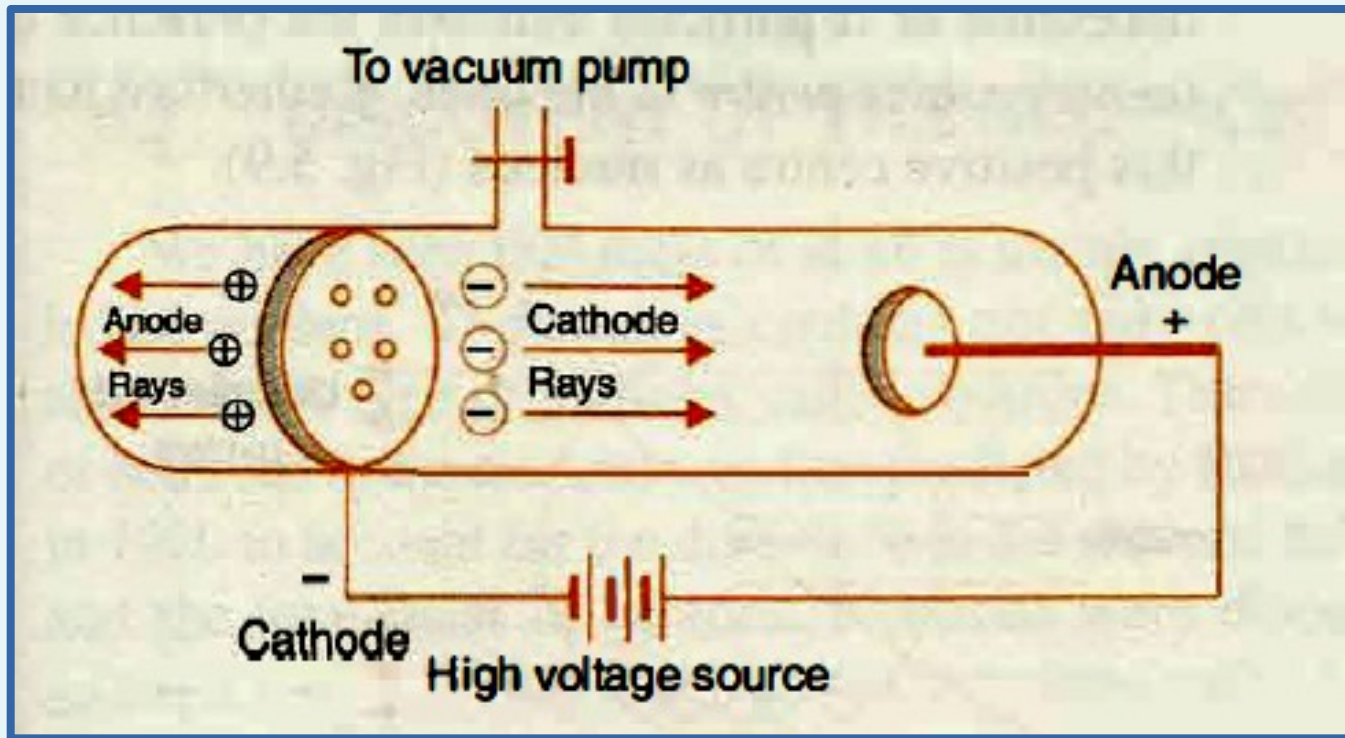
$$m = 9.1 \times 10^{-31} \text{ kg / e}^-$$

# ANODE RAYS OR CANAL RAYS

Goldstein in 1886 discovered the existence of a new type of rays in the discharge tube.



**GOLDSTEIN**



- Goldstein repeated the discharge tube experiment by using a perforated cathode.
- He evacuated the discharge tube and a high voltage is applied across the electrodes.
- He observed a new type of rays streaming behind the cathode.
- These rays were named as **anode rays or canal rays**.
- These rays travel in opposite directions to the cathode rays.



# PROPERTIES OF ANODE RAYS


- Travel in straight lines.
- Consist of material particles.
- Anode rays are positively charged.
- When a magnetic field is applied, they get deflected in the direction expected for positive particles.
- Produce heating effects.
- The  $e/m$  values of anode rays are much smaller than that of the cathode rays.

# DISCOVERY OF PROTON

- Protons were discovered by **E. Goldstein**.
- A proton is a subatomic particle having a unit positive charge and a mass nearly equal to that of hydrogen.
- **Charge of proton =  $1.602 \times 10^{-19}$  C**
- **Mass of proton =  $1.672 \times 10^{-24}$  g**

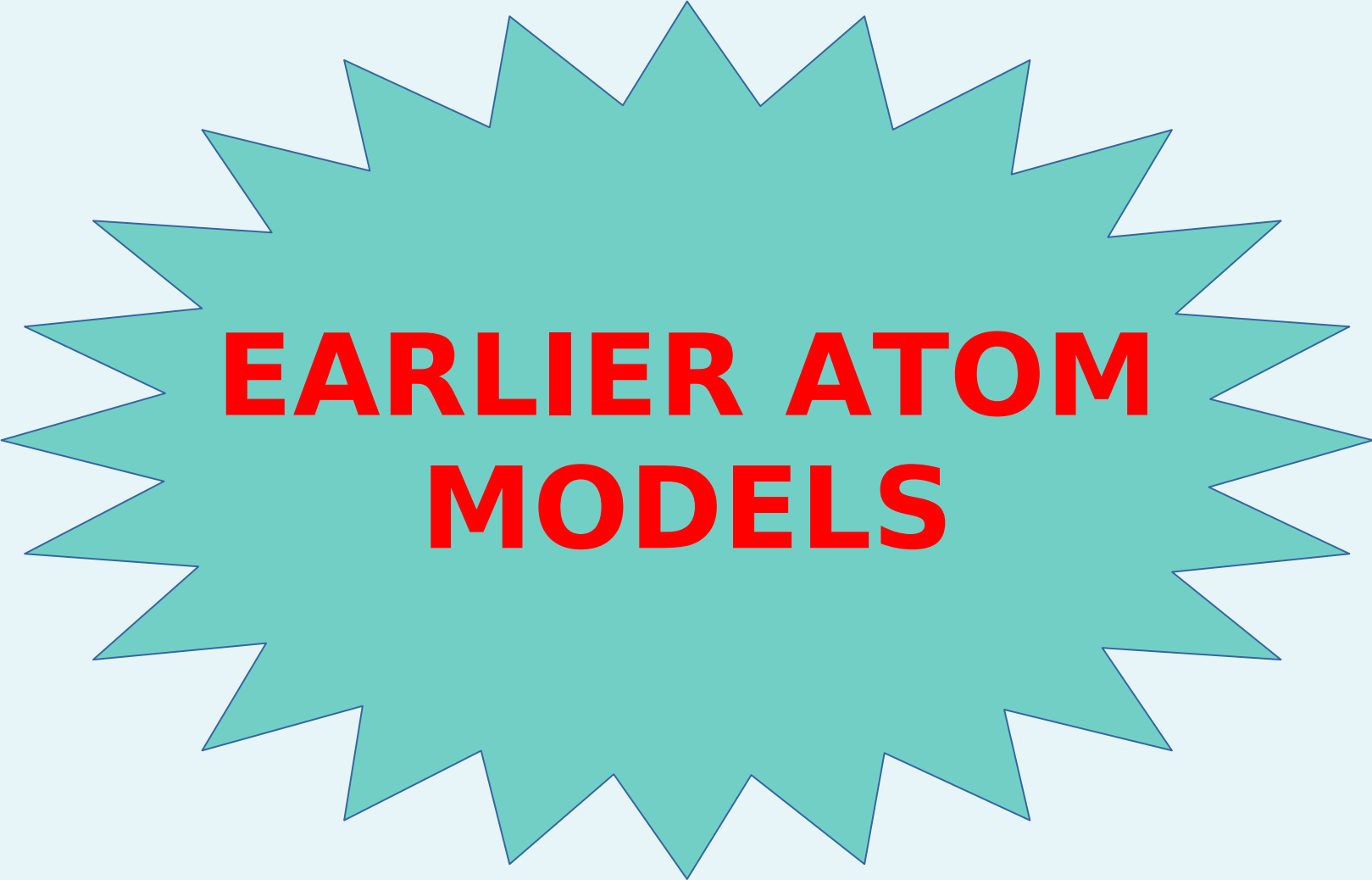

# **ORIGIN OF CATHODE RAYS AND ANODE RAYS**

- Under the influence of high electric field, the gas in the discharge tube is ionized.
- This results in the formation of particles with positive and negative charge.
- The negatively charged particles move towards the anode at very high speeds.



**→ On their way they collide with the atoms of the gas producing more electrons and positively charged particles.**

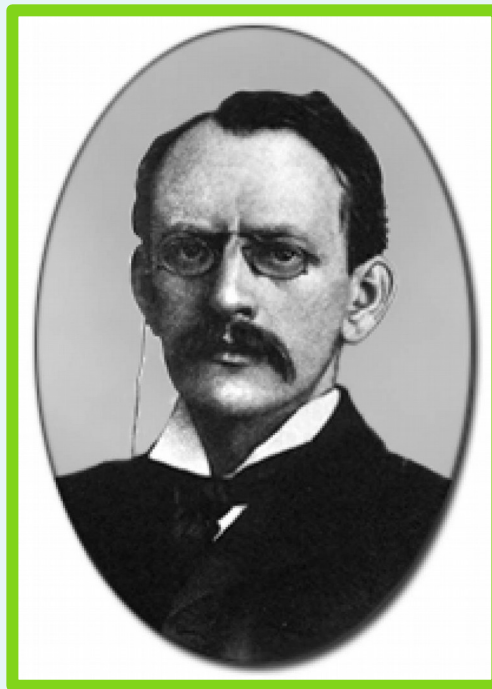
**→ The electrons moves towards the anode in the form of cathode rays while the positive ions move towards cathode in the form of anode rays.**




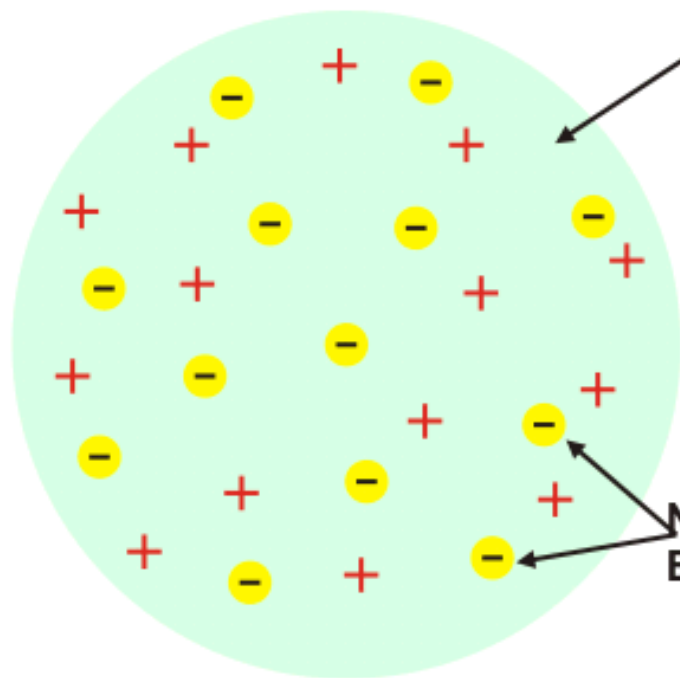
# **EARLIER ATOM MODELS**

# THOMSON'S MODEL OF ATOM

The first atom model was proposed by J.J. Thomson.



- 
- An atom may be considered as a sphere of positive charge.
  - The electrons are uniformly distributed in it to make the atom as a whole electrically neutral.
  - Therefore this atom model is known as **plum pudding model.**



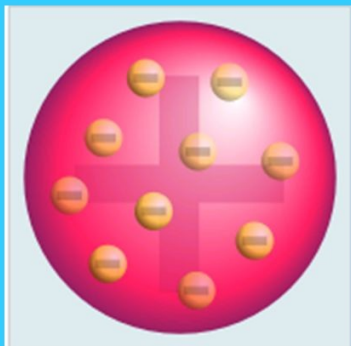
Spherical cloud of Positive Charge

Negatively Charged Electrons

**Thomson's Plum-Pudding Model**

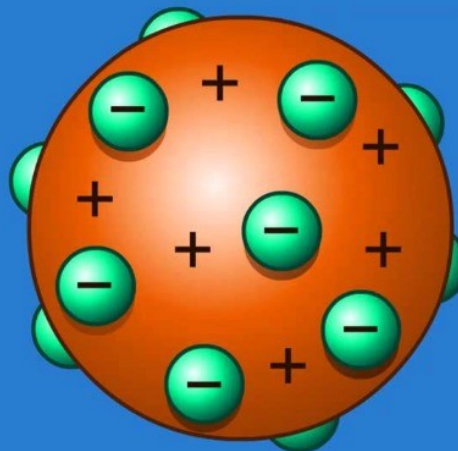


# Plum Pudding Model

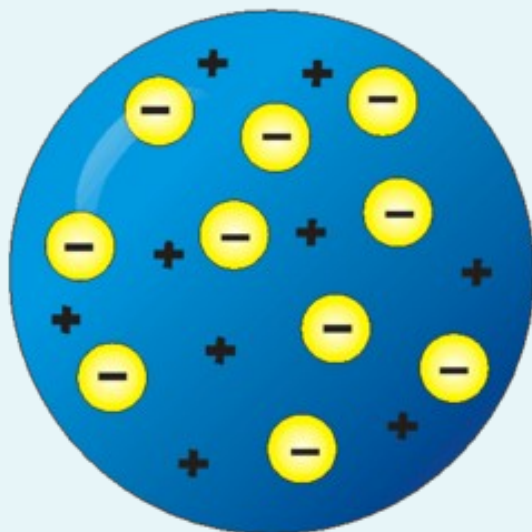
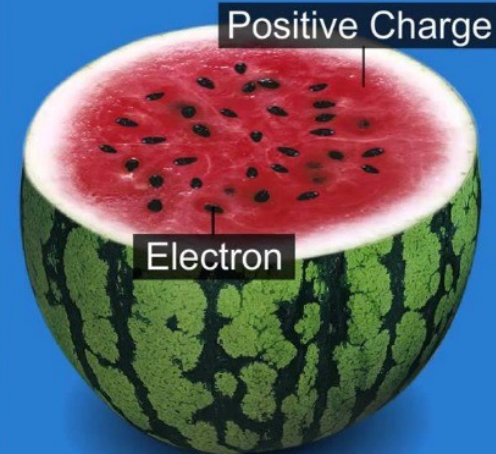


## THOMSON'S ATOMIC MODEL

Atom Model



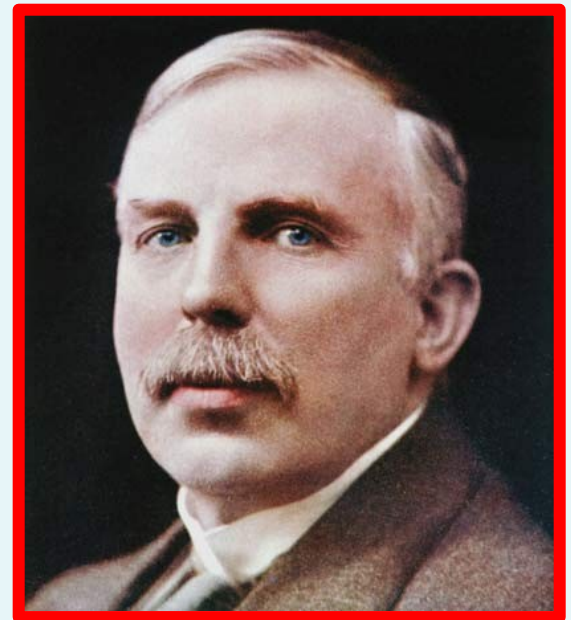
Watermelon



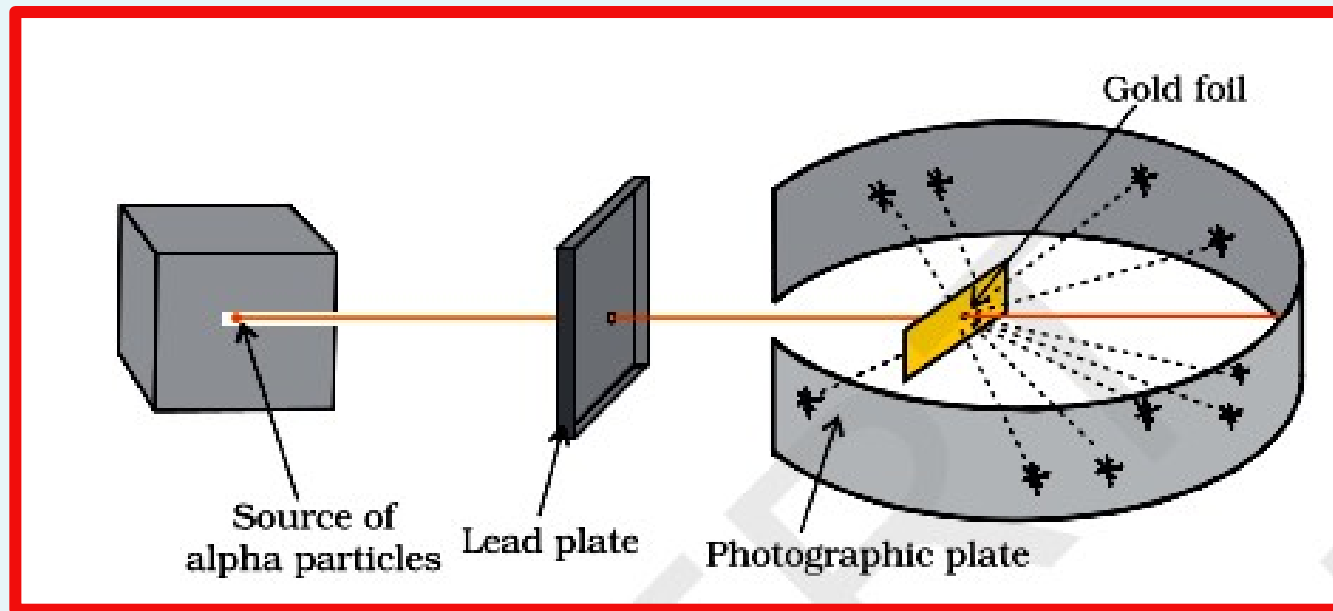
# **RUTHERFORD'S $\alpha$ -PARTICLE SCATTERING EXPERIMENT**

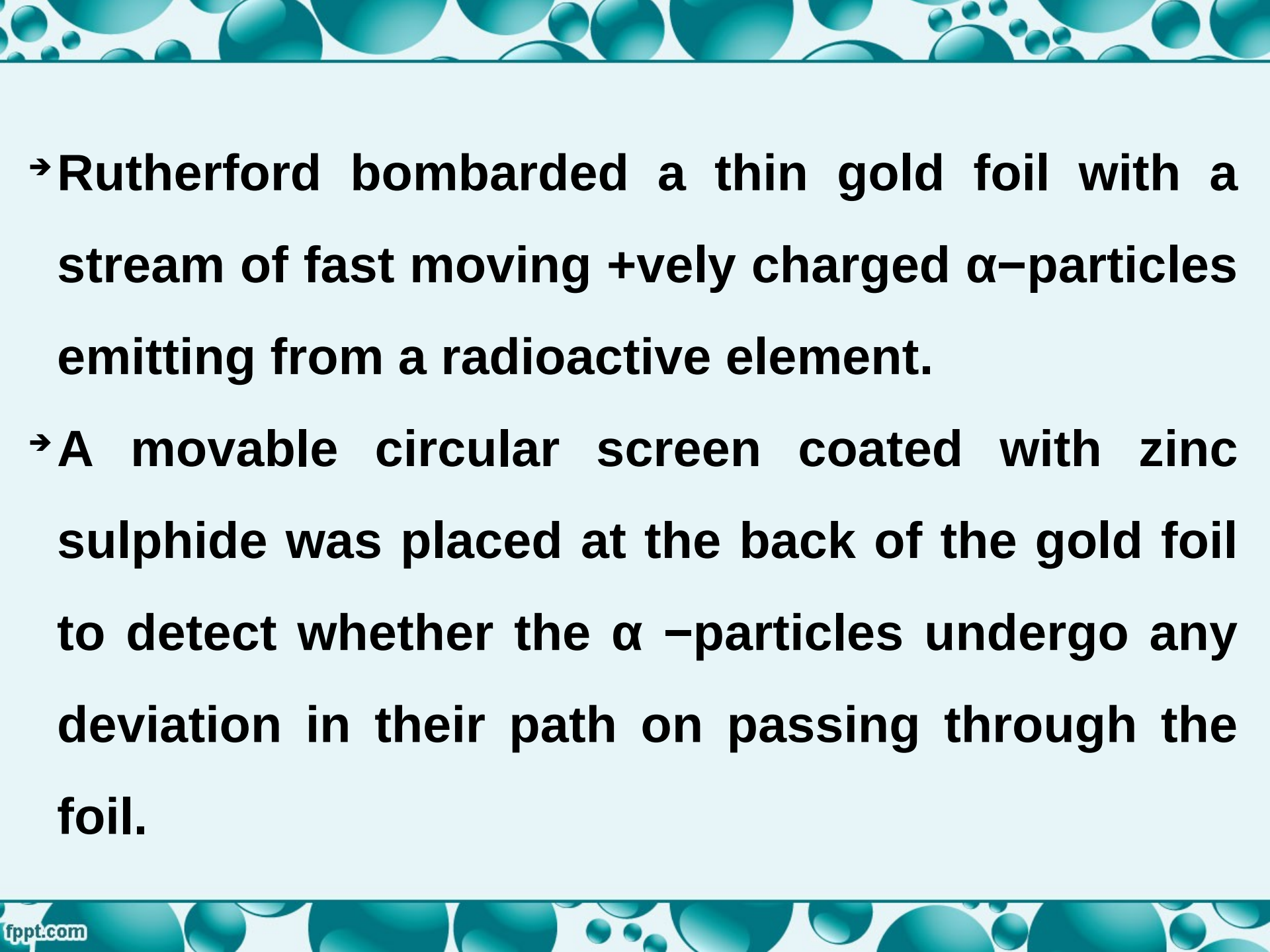
In order to find out the arrangement of electrons and protons, Rutherford in 1911 conducted a scattering experiment.

**ERNEST  
RUTHERFORD**



# EXPERIMENT




- 
- Rutherford bombarded a thin gold foil with a stream of fast moving +vely charged  $\alpha$ -particles emitting from a radioactive element.
  - A movable circular screen coated with zinc sulphide was placed at the back of the gold foil to detect whether the  $\alpha$  -particles undergo any deviation in their path on passing through the foil.

# **OBSERVATIONS**

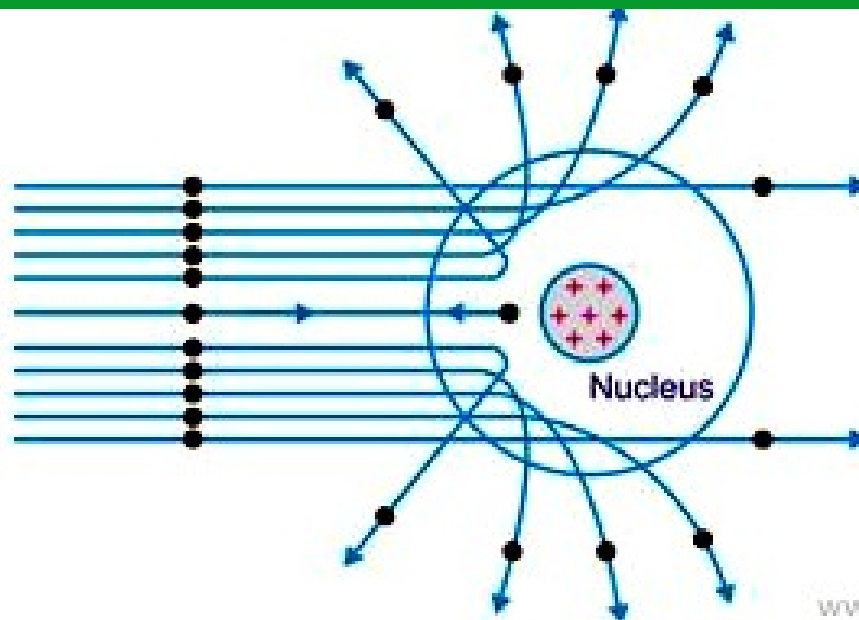
- Most of the  $\alpha$ -particles passed through the gold foil without any deviation.
- Some of the  $\alpha$  -particles were deflected by small angles.
- A very few  $\alpha$  -particles bounced back.

# CONCLUSIONS

- Since most of the  $\alpha$  -particles pass through the gold foil without any deviation, it indicates that most of the space in an atom is empty.
- $\alpha$ -particles being positively charged and having considerable mass, could be deflected only by some heavy positively charged centre.

- 
- **The small angle of deflection of  $\alpha$ -particles indicated the presence of heavy positive centre in the atom.**
  - **Rutherford named this +ve centre as nucleus.**
  - **A few of the  $\alpha$ -particles are bounced back due to the direct collision with the nucleus.**

Incident  
beam of  
 $\alpha$ -particles




[www.jee-mentor.in](http://www.jee-mentor.in)

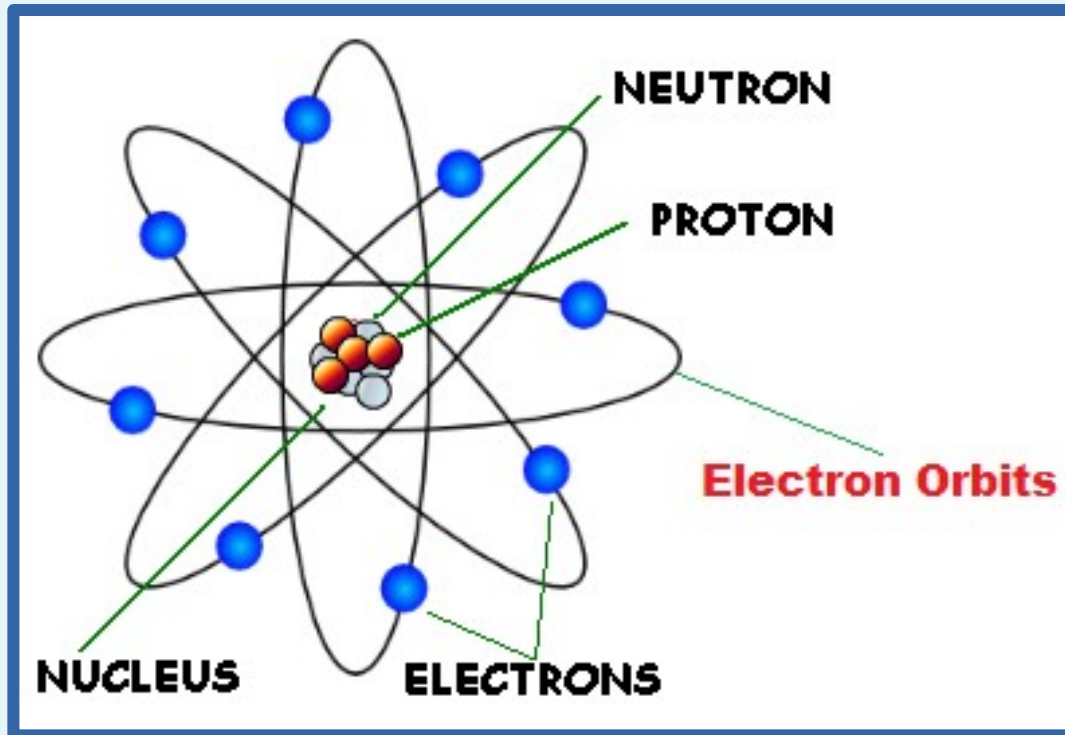


# **RUTHERFORD'S NUCLEAR MODEL OF THE ATOM**

- In an atom, the entire mass and the positive charge is concentrated in a very small region at the centre known as nucleus.
- The magnitude of the positive charge on the nucleus (number of protons) is different for different atoms.

- 
- **The nucleus is surrounded by negatively charged electrons which balance the positive charge on the nucleus.**
  - **The electrons are not stationary but are revolving around the nucleus at very high speeds.**
  - **Most of the space in an atom is empty.**

# RUTHERFORD'S ATOM MODEL



# PLANETARY MODEL OF ATOM

- Nuclear model of an atom can be compared with the solar system.
- In an atom, the electrons revolve around the nucleus like planets revolve around the sun.
- The nucleus represents the sun and the electron represents the planets.
- Therefore this model is also referred to as **planetary model of atom** and the electrons are called **planetary electrons**.

# **ATOMIC NUMBER**

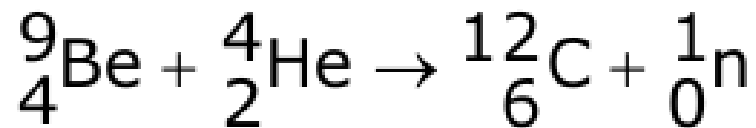
- The number of unit positive charges carried by the nucleus of an atom is termed as the atomic number.
- The atomic number is numerically equal to the number of protons present in the nucleus of the atom.
- The number of protons in an atom is equal to the number of electrons.

# DISCOVERY OF NEUTRON

Neutrons were discovered by Chadwick in 1932.



- Beryllium is bombarded with  $\alpha$ -particles.
- The emitted radiation consists of a new particle carrying no charge.
- Chadwick called the particle, neutron.



# NEUTRON

- A **neutron** is a subatomic particle having a mass equal to that of hydrogen atom and carrying no electrical charge.
- The mass of neutron is found to be  $1.675 \times 10^{-24}$  g.



# MASS NUMBER (A)

- The mass of an atom is mainly due to protons and neutrons.
- Protons and neutrons are collectively known as **nucleons**.
- The total number of protons and neutrons in the nucleus is called **mass number** of the atom.
- It is generally represented by 'A'.
- Mass number = No. of protons + Number of Neutron
- No. of Neutrons = Mass Number – Atomic Number
- i.e., **(A–Z)**

# ISOTOPES

- Atoms of an element with the same atomic number but different mass numbers are called isotopes.
- For example, hydrogen has three isotopes.
- They are Protium ( ${}^1\text{H}$ ), Deuterium ( ${}^2\text{H}$ ) and Tritium ( ${}^3\text{H}$ ).
- Carbon has three isotopes namely,  ${}^{12}\text{C}$ ,  ${}^{13}\text{C}$ ,  ${}^{14}\text{C}$ .

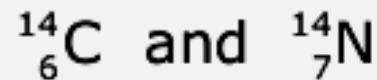
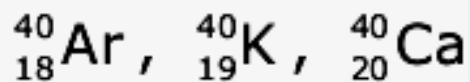
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- Carbon has three isotopes namely,  ${}^{12}\text{C}$ ,  ${}^{13}\text{C}$ ,  ${}^{14}\text{C}$ .

# ISOBARS

Atoms having the same mass number but different atomic numbers are called Isobars.

Examples



# ISOTONES

Atoms having the same number of neutrons but different mass numbers are called isotones.

**Example**



# NATURE OF ELECTROMAGNETIC RADIATIONS

## CORPUSCULAR THEORY



**NEWTON**

## **NEWTON'S CORPUSCULAR THEORY**

- Light is propagated as a stream of minute particles called corpuscles of light.
- This theory of light could explain the phenomena of reflection and refraction.
- It failed to explain the phenomena of diffraction and interference.
- Therefore the corpuscular theory was rejected.

# **ELECTROMAGNETIC RADIATIONS**

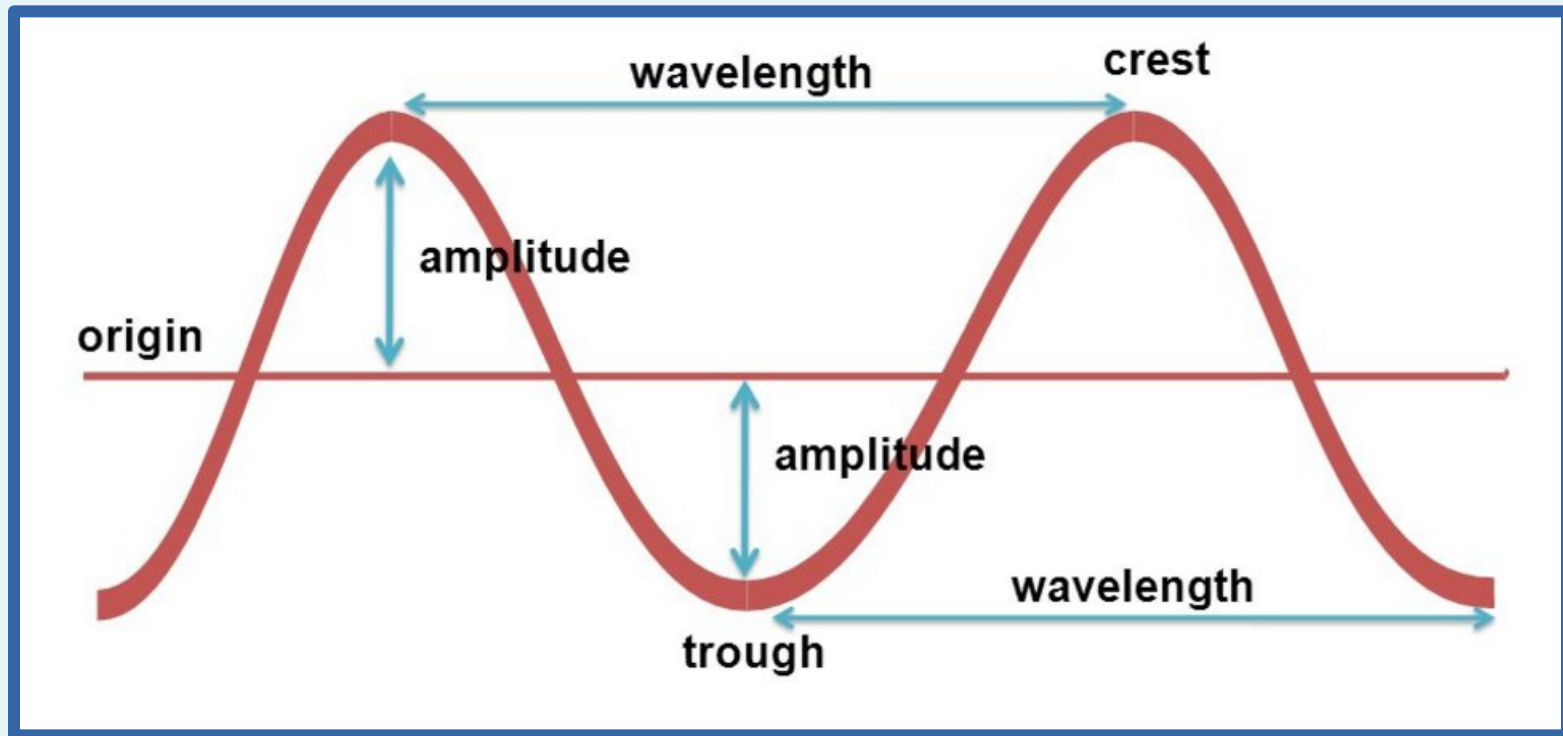
- **James Clark Maxwell in 1856 suggested that light propagates through space in the form of waves.**
- **These waves are associated with electric and magnetic fields.**
- **Therefore, these waves are called electromagnetic waves or electromagnetic radiations.**



## **CHARACTERISTICS OF ELECTROMAGNETIC RADIATIONS**

- Electromagnetic radiations propagate through space in the form of waves.
- All Electromagnetic radiations travel with a velocity of light.
- It require no medium for transmission.
- The energy of electromagnetic radiation is directly proportional to its frequency or inversely proportional to its wavelength.

# CHARACTERISTICS OF A WAVE



## **WAVE LENGTH ( $\lambda$ )**

→ The distance between two adjacent crests or troughs is called wavelength.

→ It is denoted by the Greek letter lambda ( $\lambda$ ) and is generally expressed in terms of Angstrom units.

$$1\text{\AA} = 10^{-10} \text{ m or } 10^{-8} \text{ cm}$$

# **FREQUENCY ( $\nu$ )**

- The number of waves which pass through a given point in one second is known as the frequency.
- It is denoted by the Greek letter nu ( $\nu$ ).
- The units of frequency are cycles per second or Hertz (Hz).

$$1 \text{ Hz} = 1 \text{ cycles / sec}$$

## **VELOCITY (c)**

→ The distance travelled by a wave in one second is called the velocity of a wave.

→ It is generally denoted by the letter (c).

# **AMPLITUDE (a)**

→ It is the height of the crest or depth of the trough of a wave.

→ It is generally denoted by the letter (a).

# WAVE NUMBER

- It is defined as the number of wavelengths per unit length.
- It is the inverse of wavelength.
- It is denoted by nu bar.
- It is expressed in  $\text{cm}^{-1}$  or  $\text{m}^{-1}$

$$\text{wavenumber} = \frac{1}{\text{wavelength}}$$

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

# RELATIONSHIP BETWEEN WAVELENGTH, FREQUENCY AND VELOCITY

**Velocity = Wavelength x Frequency**

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

**The velocity of electromagnetic radiations is**

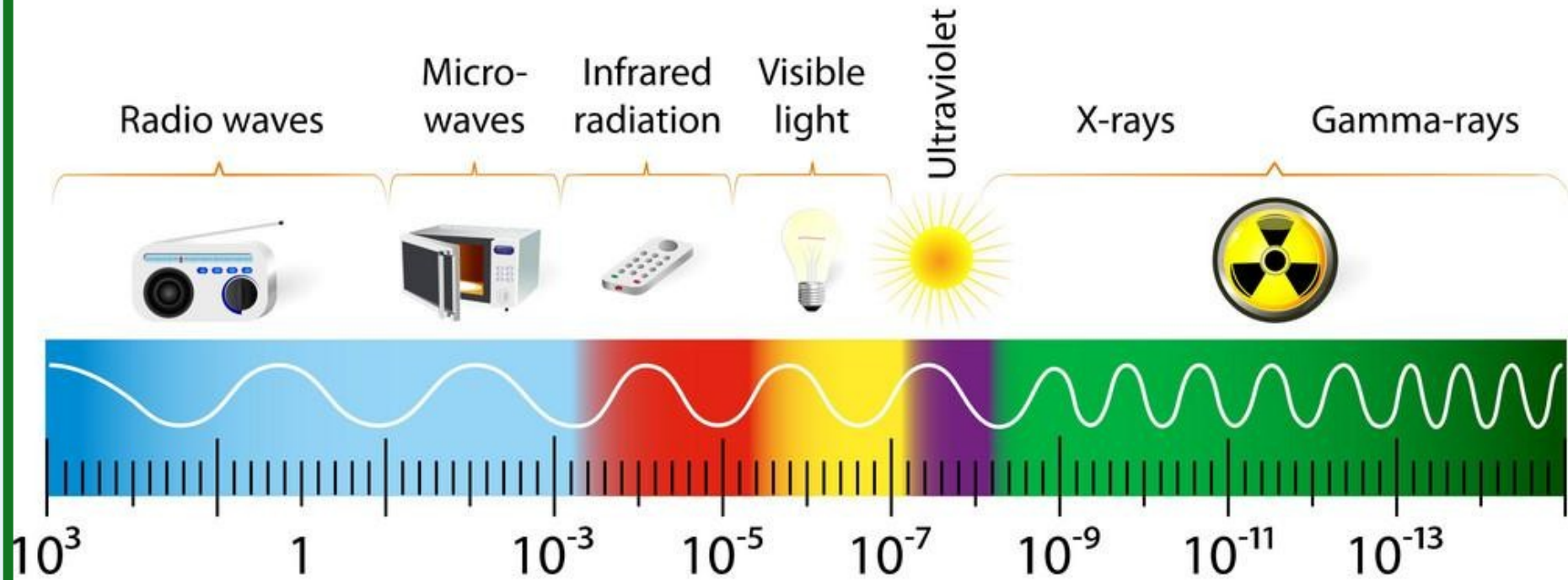
**$3 \times 10^8$  m/s.**



# ELECTROMAGNETIC SPECTRUM

The arrangement of different types of electromagnetic radiations according to the increasing wavelength or decreasing frequency is known as **electromagnetic spectrum**.

# THE ELECTROMAGNETIC SPECTRUM



→ The different regions of the electromagnetic spectrum are arranged as follows.

→ Cosmic rays,  $\gamma$ -rays, x-rays, UV region, Visible region, Infrared region, Microwaves, Radiowaves etc.

→ The wavelength of different colours constituting the visible light are as follows.

|               |               |             |              |               |               |            |      |
|---------------|---------------|-------------|--------------|---------------|---------------|------------|------|
| <b>Violet</b> | <b>Indigo</b> | <b>Blue</b> | <b>Green</b> | <b>Yellow</b> | <b>Orange</b> | <b>Red</b> |      |
| 3700          | 4300          | 4500        | 4900         | 5500          | 5900          | 6500       | 7500 |

# BLACK BODY RADIATION

→ The ideal body which emits and absorbs all frequencies is known as black body.

→ The radiation emitted by the black body is known as **black body radiation**.

# PHOTOELECTRIC EFFECT

- When a light of suitable frequency strikes a metal, electrons are ejected.
- The phenomenon is known as photoelectric effect.
- The emitted electrons are called **photoelectrons**.


**HEINRICH HERTZ**



# IMPORTANT ASPECTS

→ The ejection of electrons from the surface of a metal will take place only if the incident radiation has a certain minimum frequency.

→ The minimum frequency of light, required to cause the emission of electrons from a metal surface is called threshold frequency ( $\nu_0$ ).

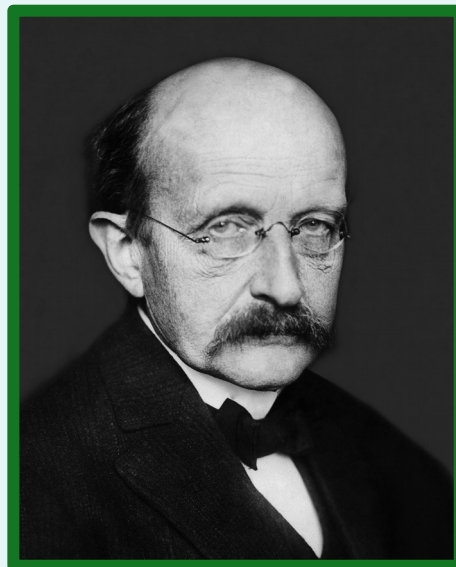


**→The kinetic energy of the ejected electrons is proportional to the frequency of the incident radiation and is independent of its intensity.**

**→The number of electrons ejected from the metal surface is proportional to the intensity of the radiation.**

# PLANCK'S QUANTUM THEORY

In order to explain the phenomena of black body radiation and photoelectric effect, Max Planck in 1900 put forward a new theory called **quantum theory** of radiation.



**MAX PLANCK**



# QUANTUM THEORY

→ Radiant energy is emitted or absorbed not continuously but discontinuously in the form of small packets of energy called **quanta**.

→ Each packet of wave is associated with a definite amount of energy. In the case of light, the quantum of energy is often called a **photon**.

**The amount of energy associated with a quantum of radiation is proportional to the frequency of radiation.**

$$E \propto \nu$$

$$E = h\nu$$

Where  $h$  is Planck's constant and is equal to  $6.626 \times 10^{-34} \text{Js}$

$$\text{But } \nu = \frac{c}{\lambda}$$

$$E = \frac{hc}{\lambda}$$

The energy is emitted or absorbed only in the integral multiple of quantum.

$$E = nh\nu$$

# **DUAL NATURE OF ELECTROMAGNETIC RADIATIONS**


- The particle nature of light could explain certain phenomena like photoelectric effect and black body radiation.
- But the phenomena such as diffraction and interference can be explained only on the basis of wave nature.
- The experimental facts suggest that light has dual character.
- i.e. particle character as well as wave character.

# **SOLAR SPECTRUM**

→ When white light is passed through a prism, it splits into a series of colour bands known as **VIBGYOR**.

→ Sunlight is composed of a collection of electromagnetic waves having different wavelengths.

→ The prism bends the light of different wavelengths to different extents.



→ The phenomenon of splitting of light into seven colours is known as **dispersion** and the series of colour bands is called a **spectrum**.

→ In this spectrum, one colour merges into the other without any gap or discontinuity. Therefore the spectrum is known as **continuous spectrum**.

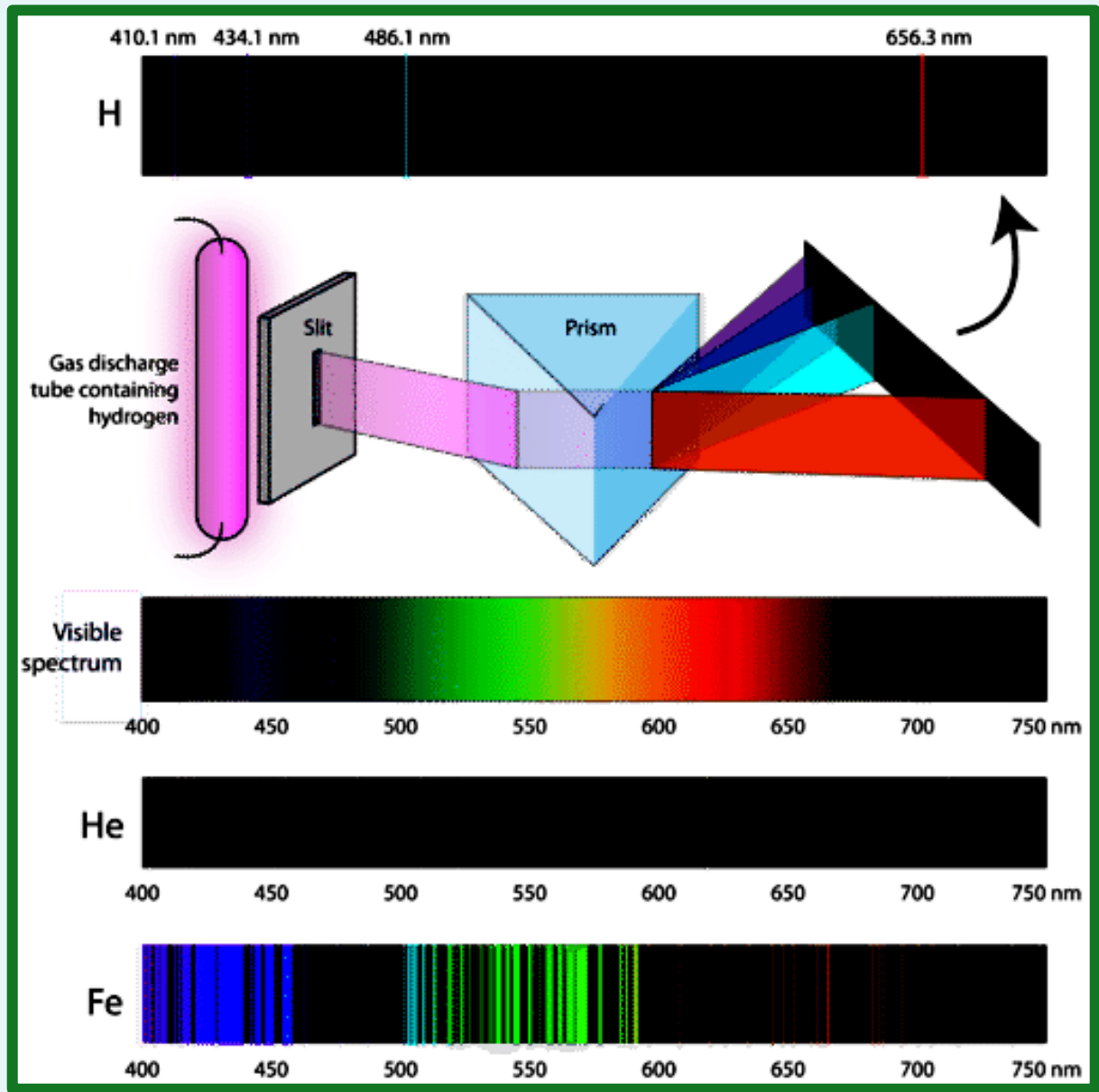
# ATOMIC SPECTRA

- The spectra of atoms are not continuous.
- The atomic spectra consist of sharp well defined lines or bands corresponding to definite wave lengths.
- Atomic spectra are of two types.
- They are Emission Spectra and Absorption Spectra.

# EMISSION SPECTRA

→ If the light emitted from an excited substance is dispersed by using an instrument called spectroscope, the spectrum obtained is not continuous but consists of a series of sharp well defined lines.

→ Each line in the spectrum corresponds to a definite wavelength.







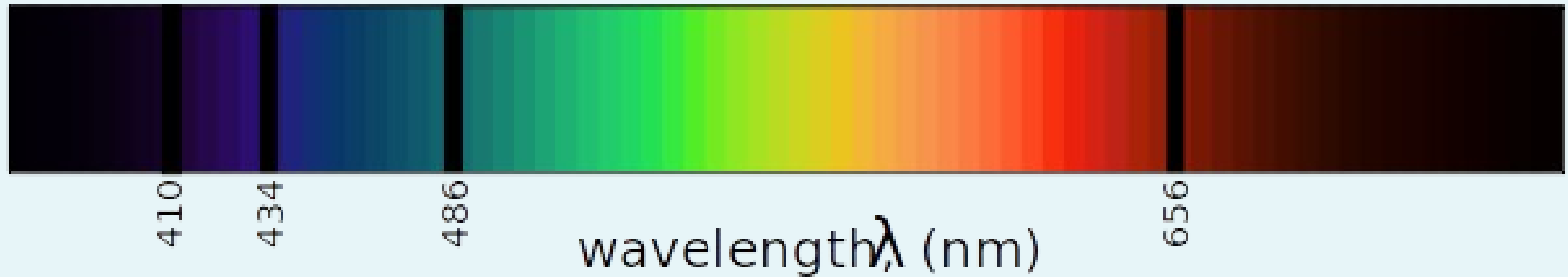
→ A spectrum containing lines of definite wavelengths is called **discontinuous spectrum** or **line spectrum**.

→ The line spectrum is also known as **atomic spectrum**.

# **ABSORPTION SPECTRA**

**When a continuous electromagnetic radiation is allowed to pass through a gas or a solution of some salt and the transmitted light is analyzed in a spectroscope, we obtain a spectrum which contains some dark lines in an otherwise continuous spectrum.**


# Hydrogen Absorption Spectrum



A spectrum containing a few dark lines due to absorption of light is known as **absorption spectrum**.

# **SPECTRUM OF HYDROGEN ATOM**

- Obtained by passing an electric discharge through hydrogen gas taken in a discharge tube under low pressure.
- The light emitted is analyzed by using a spectroscope.
- The spectrum consists of a large number of lines appearing in different region of electromagnetic spectrum.



→ Some of the lines are found in the visible region while others in ultraviolet and Infra red region.

→ The different series are Lyman Series, Balmer Series, Paschen Series, Brackett Series and Pfund Series.

→ Lyman series appear in the ultraviolet region.

→ Balmer series appear in the visible region.

→ Paschen, Brackett and Pfund series appear in the infra-red region.

# RYDBERG EQUATION

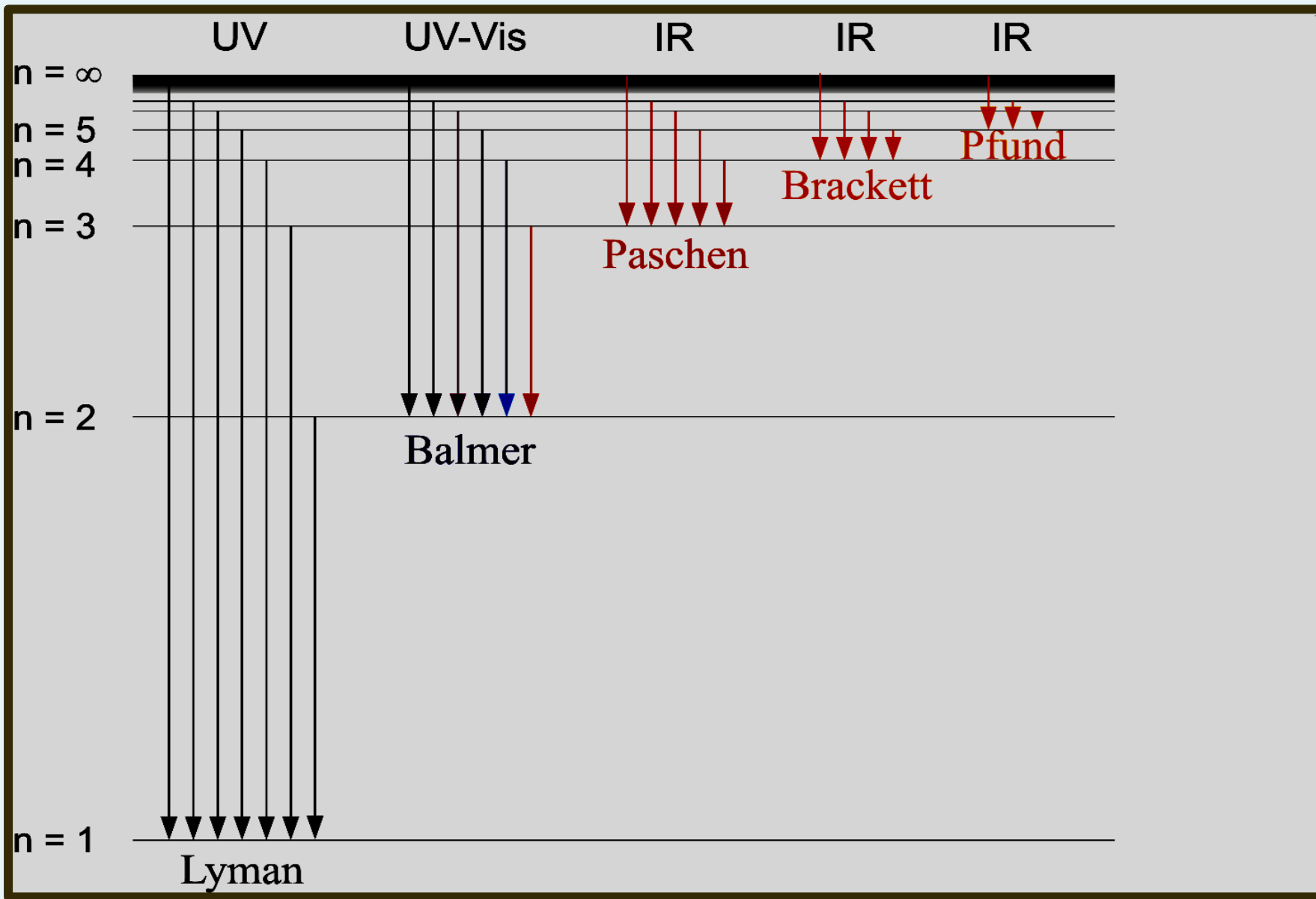
Rydberg gave a general expression which is applicable to all series of lines in the hydrogen spectrum.

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

where R is Rydberg constant.

The value of R is  $109677 \text{ cm}^{-1}$

The expression is known as **Rydberg Equation**.



### **Lyman Series**

Lyman series lies in the ultraviolet region.

$$n_1 = 1 \quad n_2 = 2, 3, 4, 5, 6, \dots$$

### **Balmer Series**

Balmer series lies in the visible region.

$$n_1 = 2 \quad n_2 = 3, 4, 5, 6, 7, \dots$$

### **Paschen Series**

Paschen series lies in the near IR region.

$$n_1 = 3 \quad n_2 = 4, 5, 6, 7, \dots$$

### **Brackett Series**

Brackett series lies in the middle IR region.

$$n_1 = 4 \quad n_2 = 5, 6, 7, \dots$$

### **Pfund Series**

Pfund series lies in the far IR region.

$$n_1 = 5 \quad n_2 = 6, 7, 8, \dots$$



# **FAILURE OF RUTHERFORD'S MODEL**

→ Rutherford's model failed to explain the stability of atoms.

→ Rutherford's model also failed to explain the existence of certain definite lines in the Hydrogen spectrum.




**→ Rutherford's atom model failed in view of electromagnetic theory proposed by Maxwell.**

**→ According to Maxwell's theory, a charged particle when accelerated emits energy in the form of electromagnetic radiations.**

**→ According to Rutherford's model, electrons are revolving around the nucleus.**

**→ This means that electrons would be in a state of acceleration all the time.**

- 
- Since electrons are charged particles, the electrons revolving in an orbit should continuously emit radiations.**
  - As a result, it would slow down and would no longer be able to withstand the attractive force of the nucleus.**
  - Hence it would move closer and closer to the nucleus and would finally fall into the nucleus by following a spiral path.**
  - But we know that an atom is stable.**
  - Thus Rutherford's model failed to explain the stability of atoms.**

# BOHR MODEL OF THE ATOM

In 1913, Niels Bohr proposed a model of the atom which was based upon the Planck's Quantum theory of radiation.



**NIEL'S BOHR**

→The electrons in an atom revolve around the nucleus in certain selected circular paths called orbits.

→As long as an electron revolves in a particular orbit, it does not lose or gain energy.

→Therefore, these orbits are also called stationary orbits.

→Only those orbits are permitted in which the angular momentum ( $mvr$ ) of the electron is an integral multiple

of  $\frac{h}{2\pi}$  i.e.,  $mvr = \frac{nh}{2\pi}$

→When an electron jumps from one orbit to another, it will absorb or emit radiation of a definite frequency.

when an electron jumps from a lower level to a higher level, it absorbs energy equal to  $E_2 - E_1$ .

When the electron jumps back to the lower level, it emits the same amount of energy.

$$\Delta E = E_2 - E_1 = h\nu$$


$$\nu = \frac{E_2 - E_1}{h}$$

This amount of energy absorbed or emitted is given by the difference in energies of the two levels concerned.

# MERITS OF BOHR MODEL

- Bohr model could explain the stability of an atom.
- Bohr's theory helped in calculating the energy of the electron in a particular orbit of hydrogen atom.
- Bohr's theory helped in calculating the radius of each circular orbit by using the expression

$$r_n = 0.529 \times n^2 \text{ where } n = 1, 2, 3, \dots$$



**→ Bohr model could explain the line spectrum of hydrogen.**

**→ Bohr model could explain the simultaneous appearance of a large number of lines in the hydrogen spectrum.**



# DEMERITS OF BOHR MODEL

- It could not explain the line spectrum of multi electron atoms.
- It could not explain the splitting of spectral lines under the influence of magnetic field (**Zeeman effect**) and electric field (**Stark effect**).
- It could not explain the shape of molecules formed by the combination of atoms.
- Bohr model could not explain the fine structure of the spectral lines produced by hydrogen.

# DE-BROGLIE EQUATION

According to de-Broglie, the wave length ( $\lambda$ ) associated with a particle of mass 'm' moving with velocity (v) is given by the relation

$$\lambda = \frac{h}{mv} \quad \text{or} \quad \lambda = \frac{h}{P} \quad [P = mv]$$

Where ' $\lambda$ ' is the wavelength, 'h' is Planck's constant, 'P' is the momentum.

# DERIVATION OF DE-BROGLIE RELATIONSHIP

Consider a photon of light energy,  $E$ . According to Max Planck,

$$E = h\nu \dots \dots \dots (1)$$

where  $\nu$  is the frequency,  $h$  is the Planck's constant.

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

$$E = \frac{hc}{\lambda} \dots \dots \dots (2)$$

According to Einstein's mass energy relationship

$$E = mc^2 \dots \dots \dots (3)$$

Combining equations (2) and (3), we get

$$\frac{hc}{\lambda} = mc^2$$

$$\frac{h}{\lambda} = mc$$

$$\lambda = \frac{h}{mc}$$

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

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

Where  $P = mv$  is the momentum.

This equation is known as **de-Broglie equation** and  $\lambda$  is called **de-Broglie wave length**.

# HEISENBERG'S UNCERTAINTY PRINCIPLE

Heisenberg in 1927, pointed out that we cannot measure accurately both the position and velocity of a particle as small as electron.



**WERNER HEISENBERG**

→“It is impossible to measure simultaneously both the position and velocity of a microscopic particle in motion with absolute accuracy”.

→Mathematically it can be expressed as

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

→Where  $\Delta x$  is the uncertainty in position and  $\Delta p$  is the uncertainty in momentum.

# QUANTUM MECHANICS


Quantum mechanics was developed independently in 1926 by Werner Heisenberg and Erwin Schrodinger



**WERNER HEISENBER**



**& ERWIN SCHRODINGER**



→ **The branch of science that takes into account, the dual behaviour of matter is called Quantum mechanics.**

→ **Quantum mechanics is a theoretical science that deals with the study of the motions of the microscopic objects that have the observable wave like and particle like properties.**



# SCHRODINGER WAVE EQUATION

On the basis of de-Broglie concept of matter waves and Heisenberg's uncertainty principle, a new model of atom was developed, known as **quantum mechanical model**.

In this model, the behaviour of the electron in an atom is described by an equation known as **Schrodinger Wave Equation**.

## Schrodinger equation is represented as

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

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

Where x, y and z are three Cartesian coordinates, E is the total energy, V is the potential energy, m is the mass of the electron, h is Planck's constant and  $\Psi$  is the amplitude of the electron wave.

→ For a system such as an atom or a molecule whose energy does not change with time, the Schrodinger equation is written as  $H \Psi = E \Psi$

→ Where H is a mathematical operator called **Hamiltonian Operator.**

# SIGNIFICANCE OF $\Psi$

- $\Psi$  is the amplitude of the electron wave.
- $\Psi$  has no physical significance.
- Its square i.e.,  $\Psi^2$  has a physical significance.
- $\Psi^2$  gives the intensity of the electron at any point.
- In other words,  $\Psi^2$  gives the probability of finding an electron in a given region around the nucleus.
- Thus  $\Psi^2$  is termed as probability density and  $\Psi$  is called probability amplitude.

# ORBITAL

- An orbital may be defined as the region of space around the nucleus where the probability of finding the electron is maximum.
- Each orbital has definite amount of energy.


# DIFFERENCE BETWEEN AN ORBIT AND AN ORBITAL

| Orbit    |   | Orbital  |   |
|----------|---|----------|---|
| <b>1</b> | An orbit is a well defined circular path followed by the revolving electron around the nucleus. | <b>1</b> | An orbital is a region of space around the nucleus of an atom where there is a high probability of finding an electron. |
| <b>2</b> | It represents the planar motion of an electron  | <b>2</b> | It represents the three dimensional motion of an electron around the nucleus.   |
| <b>3</b> | The maximum number of electrons in an orbit is $2n^2$   | <b>3</b> | An orbital cannot accommodate more than 2 electrons.  |
| <b>4</b> | Orbits are circular in shape  | <b>4</b> | Orbitals have different shapes. s orbitals are spherical, p orbitals are dumbbell shaped.                               |
| <b>5</b> | Concept of well defined orbits is against Heisenberg's uncertainty principle                    | <b>5</b> | Concept of orbital is in accordance with Heisenberg's uncertainty principle.  |

# QUANTUM NUMBERS

→ In an atom, the orbitals are designated by a set of numbers known as quantum numbers.

→ In order to specify energy, size, shape and orientation of the electron orbital, three quantum numbers are required.



**→ In order to designate the electron, an additional quantum number, called spin quantum number is required.**

**→ Thus each orbital in an atom is designated by a set of three quantum numbers and each electron is designated by a set of four quantum numbers.**





**The different quantum numbers are**

**1. Principal Quantum Number (n)**


**2. Angular Momentum Quantum Number (l)**

**3. Magnetic Quantum Number (m)**

**4. Spin Quantum Number (s)**

# PRINCIPAL QUANTUM NUMBER

- Principal quantum number is denoted by the letter 'n'.
- It represents the main shell.
- It determines the energy of an electron.
- This quantum number tells us in which principal energy level, the electron is present.



**→ It can have any whole number value such as 1,2,3,4 ..... corresponding to K, L, M, N...**

**→ As the value of 'n' increases, the electron gets farther away from the nucleus.**

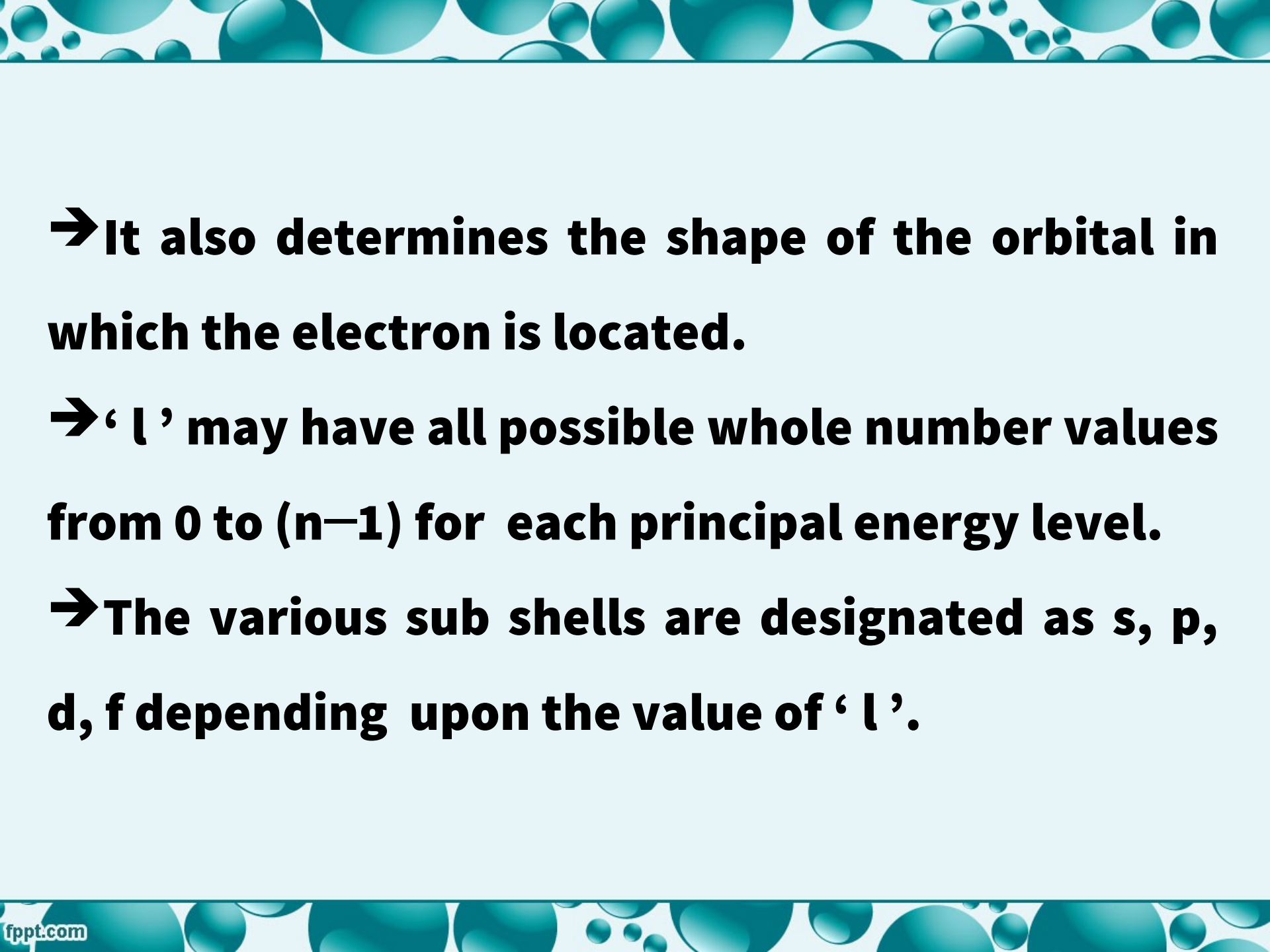
**→ Principal quantum number also determines the size of the orbital.**

**ANGULAR MOMENTUM QUANTUM NUMBER  
or  
AZIMUTHAL QUANTUM NUMBER ( l )**

→ This is denoted by 'l'.

→ This quantum number determines the angular momentum of the electron.

→ The value of 'l' gives the sub shell in which the electron is located.

- 
- It also determines the shape of the orbital in which the electron is located.**
  - ‘ l ’ may have all possible whole number values from 0 to (n–1) for each principal energy level.**
  - The various sub shells are designated as s, p, d, f depending upon the value of ‘ l ’.**

**→ For  $n = 1$ , 'l' can have only one value. i.e., 0.**

**→ It means that electron present in the first energy level can be present only in the s sub shell. i.e., 1s.**

**→ For  $n = 2$ , 'l' can have only two values. i.e., 0 and 1.**

**→ It means that electron present in the second principal energy level may be located either in the s sub shell or p sub shell. i.e., 2s and 2p.**

**→ For  $n = 3$ , 'l' can have only three values.**

**→ i.e., 0, 1 and 2.**

**→ It means that electron present in the third principal energy level may be located either in the s sub shell, p sub shell or d sub shell.**

**→ i.e., 3s, 3p and 3d.**

# MAGNETIC QUANTUM NUMBER

- This quantum number is denoted by 'm'.
- It represents the different orientations of electron cloud in a particular sub shell.
- These different orientations are called orbitals.
- Magnetic quantum number represents the number of orbitals present in the sub shell.
- The possible values of 'm' ranges from -l to +l including zero or 'm' can have  $(2l + 1)$  values.



→ For  $l = 0$ ,  $m$  can have one value,  $m = 0$ , It implies that s sub shell has only one orbital.

→ For  $l = 1$ ,  $m$  can have three values,  $m = -1, 0, +1$ . It implies that p sub shell has three orbitals.

→ For  $l = 2$ ,  $m$  can have five values,  $m = -2, -1, 0, +1, +2$ . It implies that d sub shell has five orbitals.

→ For  $l = 3$ ,  $m$  can have seven value,  $m = -3, -2, -1, 0, +1, +2, +3$ .

→ It implies that f sub shell has seven orbitals.

# SPIN QUANTUM NUMBER

- It tells us about the direction of spin of the electron.
- i.e., clockwise or anticlockwise.
- The spin quantum number can have only two values,  $+1/2$  and  $-1/2$ .
- The value  $+1/2$  indicates clockwise spin and the value  $-1/2$  indicates anticlockwise spin.



# **SHAPES OF ORBITALS**

# **s - ORBITALS**

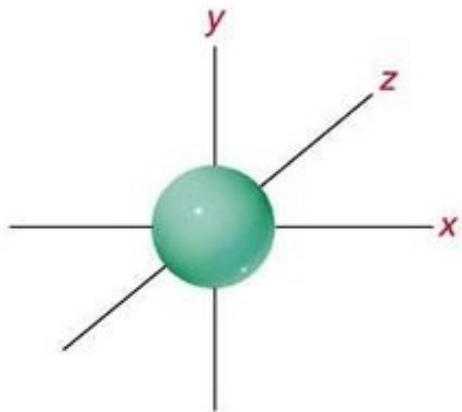
For s-orbitals,  $l = 0$  and hence  $m$  can have only one value i.e.,  $m = 0$ .

→ This means that the probability of finding the electron in s-orbitals is same in all directions.

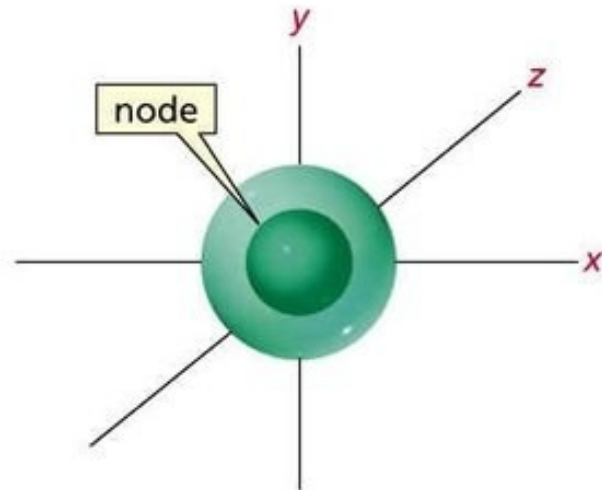
→ In other words, s-orbitals are spherically symmetrical.

→ In the case of 2s orbitals, there is a spherical shell where the electron density is zero.

→ This is called a node.



1s atomic orbital



2s atomic orbital

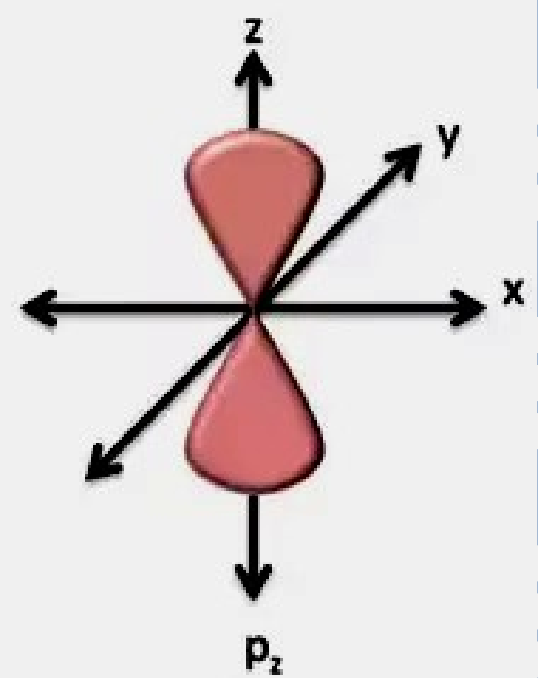
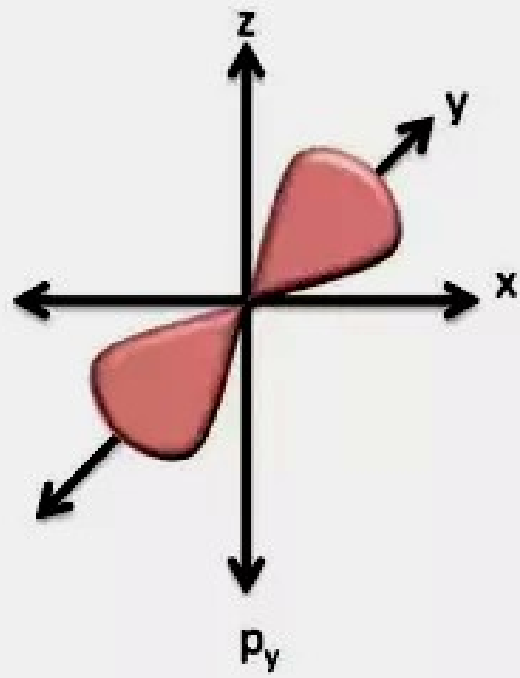
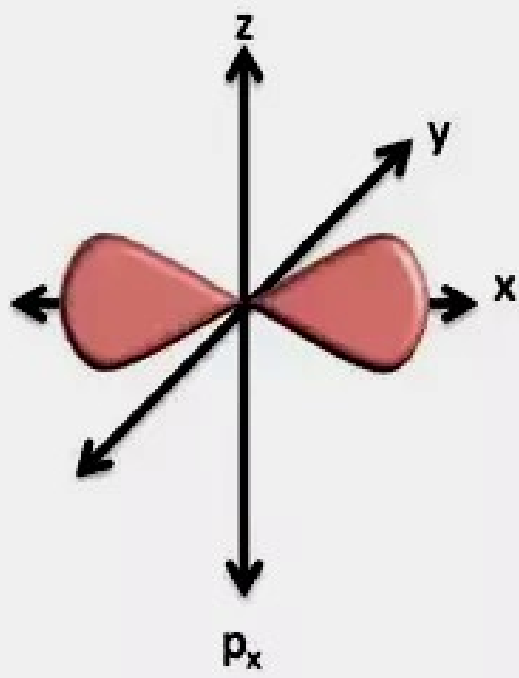
# **p - ORBITALS**

For p-orbitals,  $l = 1$  and hence  $m$  can have 3 values i.e.,  $m = -1, 0, +1$ .

→ This means that there are three p orbitals in each p sub shell.

→ These are designated as  $P_x$ ,  $P_y$  and  $P_z$ .

→ P orbitals are dumb bell shaped.



# **d - ORBITALS**

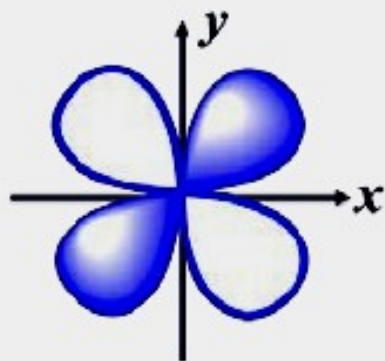
→ For d-orbitals,  $l = 2$  and hence  $m$  can have 5 values i.e.,  $m = +2, +1, 0, -1, -2$ .

→ This means that there are five d orbitals in each d sub shell.

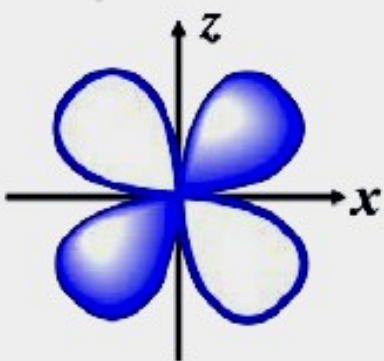
→ These are designated as  $d_{xy}$  ,  $d_{xz}$  ,  $d_{yz}$  ,  $d_{x^2-y^2}$  and  $d_{z^2}$  .

→ d orbitals are double dumb bell shaped.

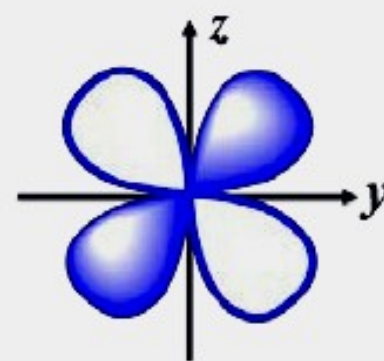




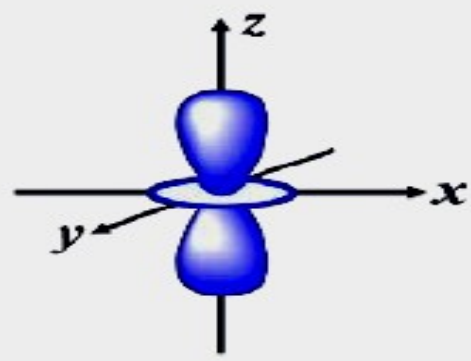
$d_{xy}$



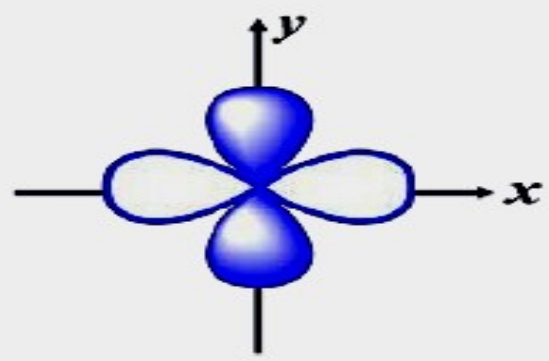
$d_{xz}$



$d_{yz}$



$d_{z^2}$



$x^2-y^2$



# **Rules for filling of orbitals in an atom**

# PAULI'S EXCLUSION PRINCIPLE

“No two electrons in an atom can have the same values for all the four quantum numbers”.

Thus in any atom, the two electrons may have a maximum of three quantum numbers the same, but the fourth must be different.

Eg:- Consider K shell where  $n = 1$ .

$$n = 1 \quad l = 0 \quad m = 0 \quad s = +1/2$$

$$n = 1 \quad l = 0 \quad m = 0 \quad s = -1/2$$

# NOTE

→ On the basis of Pauli's Exclusion Principle, it is concluded that an orbital can have a maximum of two electrons and they must have opposite spins.

→ s-subshell can have a maximum of 2 electrons

→ p-subshell can have a maximum of 6 electrons

→ d-subshell can have a maximum of 10 electrons

→ f-subshell can have a maximum of 14 electrons

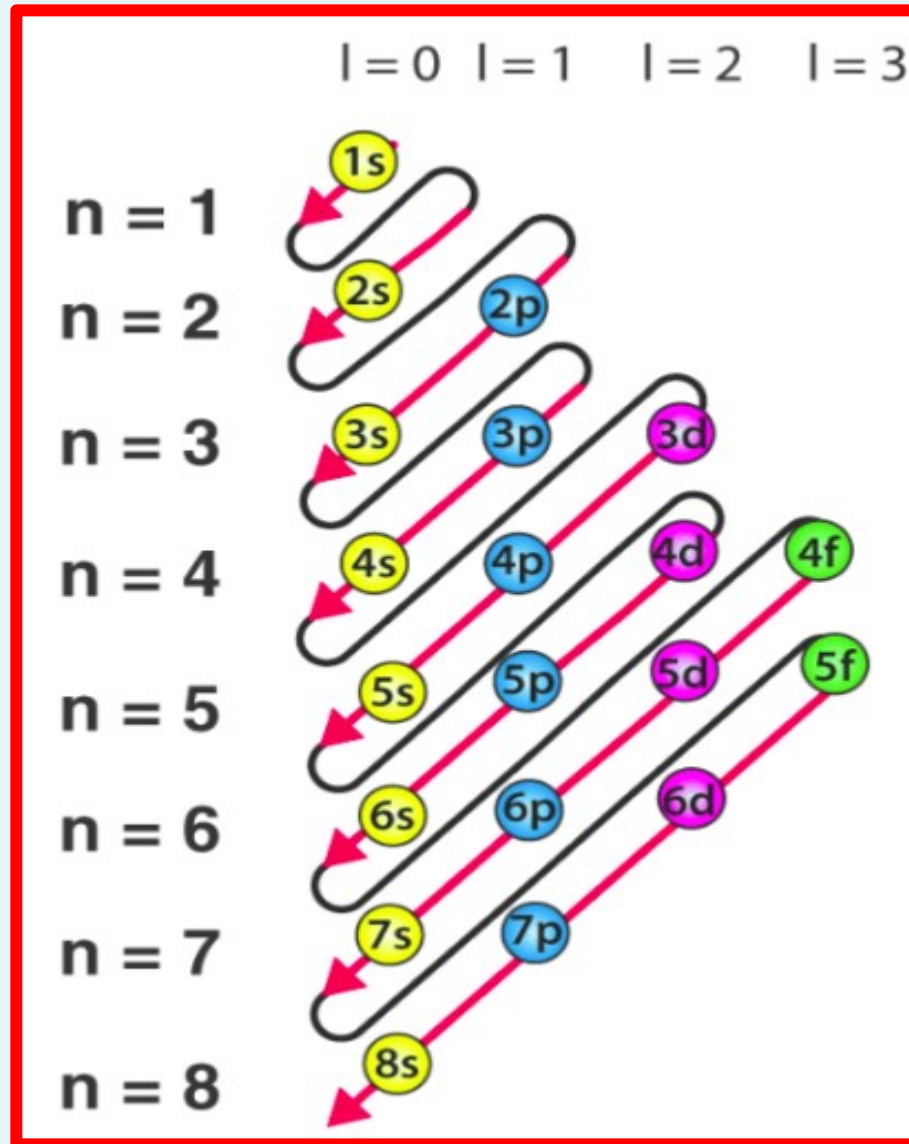
# AUFBAU PRINCIPLE

According to Aufbau Principle, the electrons are filled in various orbitals in the increasing order of their energies.

The increasing order of energies of various orbital is

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

.....



# **(n + l) RULE**

→ Orbitals are filled in the order of increasing value of  $(n + l)$ .

→ Eg:- 4s ( $n + l = 4 + 0 = 4$ ) is filled before 3d ( $n + l = 3 + 2 = 5$ )

→ If two orbitals have the same  $(n + l)$  value, the one with lower 'n' value will be filled first.

→ Eg:- 2p ( $n + l = 2 + 1 = 3$ ) is filled before 3s ( $n + l = 3 + 0 = 3$ )

because 2p has lower value of n.

# HUND'S RULE OF MAXIMUM MULTIPLICITY

**Hund's Rule** states that electron pairing will not take place in orbitals of same energy until each orbital is first singly filled with parallel spin.



# **ELECTRONIC CONFIGURATION**

- It is the distribution of electrons in the various orbitals of the atom.
- The number of electrons in an atom will be equal to the atomic number.
- These electrons are placed in the various orbitals in the increasing order of energy.

# EXAMPLES

| Atomic Number | Element   | Electronic Configuration         |
|---------------|-----------|----------------------------------|
| 1             | Hydrogen  | $1s^1$                           |
| 2             | Helium    | $1s^2$                           |
| 3             | Lithium   | $1s^2 2s^1$                      |
| 4             | Beryllium | $1s^2 2s^2$                      |
| 5             | Boron     | $1s^2 2s^2 2p_x^1$               |
| 6             | Carbon    | $1s^2 2s^2 2p_x^1 2p_y^1$        |
| 7             | Nitrogen  | $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$ |
| 8             | Oxygen    | $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$ |
| 9             | Fluorine  | $1s^2 2s^2 2p_x^2 2p_y^2 2p_z^1$ |
| 10            | Neon      | $1s^2 2s^2 2p_x^2 2p_y^2 2p_z^2$ |

**THANK YOU**

