Chapter # 02

Atomic Structure

Major Concepts

2.1 Discharge Tube Experiment
2.2 Planck's Quantum Theory
2.3 Bohr's Atomic Model
2.4 X-Rays
2.5 Quantum Numbers and Orbitals
2.6 Electronic Configurations

Learing out comes

The students will be able to:

- Summarize Bohr's atomic theory. (Applying)
- Use Bohr's model for calculating radii of orbits. (Understanding)
- Use Bohr's atomic model for calculating energy of electron in a given orbit hydrogen atom.
- Relate energy equation (for electron) to frequency, wave length, and wave numb of radiation emitted or absorbed by electron.
- Explain production, properties, types and uses of X-rays.(Understanding)
- Define photon as a unit of radiation energy.(Remembering)
- Describe the concept of orbitals. (Understanding)
- Explain the significance of quantized energies of electrons.(Applying)
- Distinguish among principal energy levels, energy sub levels, and atom orbitals. (Understanding)
- Describe the general shapes of s, p, and d-orbitals.(Understanding)
- Relate the discrete line spectrum of hydrogen to energy levels of electrons in t hydrogen atom. (Applying)
- Describe the hydrogen atom using the Quantum theory.(Understanding)
- Use the Auf bau Principle, Pauli Exclusion Principle and Hund's Rule to write t electronic configuration of the elements.(Applying)
- Describes the orbitals of hydrogen atom in order of increasi energy. (Understanding)
- Explain the sequence of filling of electrons in many electron atoms.(Applying) Write electronic configuration of atoms.(Applying)

Introduction

We know that universe is made of matter. All the matter is composed of atoms. It means that everything before you is composed of very small particles which cannot be seen by you. The water we drink, the food we eat, the cloths we wear, the air we breathe, the chair you are sitting on, the trees swaying in the invisible breeze, the rivers, the high mountains you are climbing on, the seashores you are enjoying a lot, the flowers that give you a lot of fragrance, the daily life items we use, the shining stars, even you and I are composed of these tiny particles. The idea that matter is made up of fundamental particles called atoms is known as the atomic theory of matter.

The History of Atomic Theory

The theory of the atom has had a long history. The Greek philosopher Democritus was among the first who described the material world as made up of tiny indivisible particles which he called atoms, derived from the Greek word atomos, meaning "uncutable" or "indivisible". This hypothesis was not based on scientific observations. The idea of Democritus was not accepted by Plato and Aristotle, the Scientist of the same time.

In 1803, John Dalton, an English school teacher, chemist, meteorologist, and physicist proposed the first modern theory of the atom which was experimental based. He is best known for his pioneering work in the development of modern atomic theory, and his research into color blindness. He postulated that all matter is made of extremely small particles, called atoms, and that all atoms of a given element are identical, but they are different from atoms of all other elements.


John Dalton
(1766-1844)

On the basis of Dalton's atomic theory, the atom can be defined as the basic unit of an element that can enter into chemical reaction. In this regard, he is recognized as the father of the atomic theory. However, this theory raised more questions and a series of investigations, in the late 19th century, began to suggest that atoms are made up of even smaller particles which are called subatomic particles. These particles include electron, proton, neutron, positron, neutrino etc. The arrangement of these particles within an atom determines its physical and chemical properties as well as its structure.

2.1 Discharge Tube Experiment

William Crookes, a British physicist, and other scientists designed the discharge tubes which were called the Crookes discharges tubes or cathode rays tubes. This discharge tube was later slightly modified by J. J. Thomson. The Crooks tube was used by Crookes in a number of experiments and was later used in experiments leading to the discovery of protons by Gold Stein (1886), X-rays by W. C. Roentgen (1895) and of the electron by J. J. Thomson (1897).

William Crookes
(1832 - 1919)

Construction of Discharge tube

Discharge tube (cathode rays tube) is a thick walled glass tube from which most of the air has been evacuated. It has two me electrodes (negatively charged electrode, cathode and positively charged electrod anode).It is also connected to a vacuum pump to reduce pressure inside the tube. It filled with a gas, air or vapours of a substance under low pressure (10 torr). Th electrodes of this tube are attached to a high voltage battery (5000-10000 V).

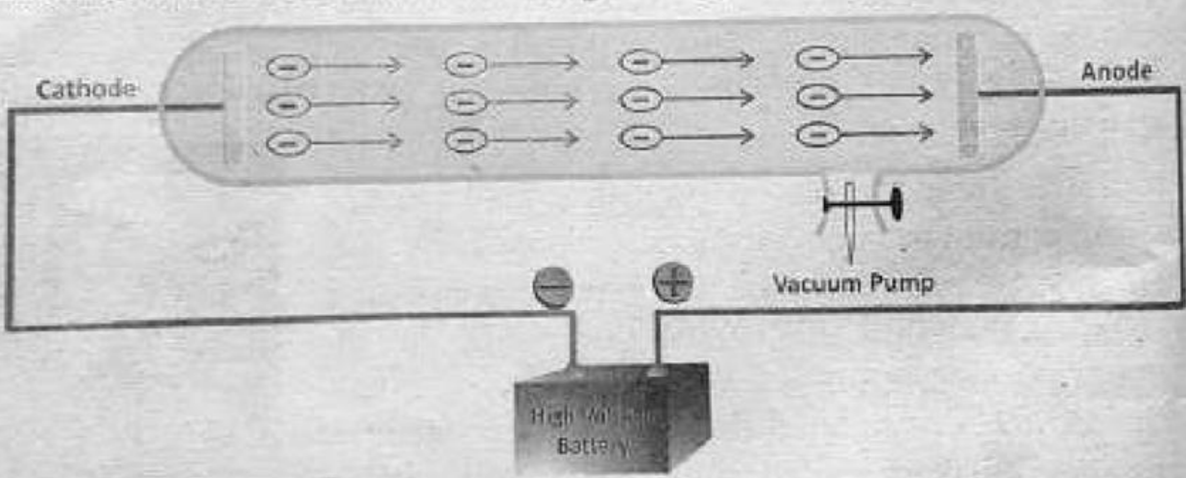

Figure 2.1: Discharge tube (cathode rays tube)

2.1.1 Cathodes rays-Discovery of the Electron

The electric current cannot pass through gases at ordinary pressure. When press inside the tube is reduced and high voltage is applied, then the gas begins to cond electric current by producing a uniform glow inside the tube. The colour of gl depends on the nature of gas and also depends on the material of glass tube. In discharge tube, the helium gas glows with pink colour while neon glows with orange red colour. When pressure is further reduced to 0.01 torr, glow disappe and some invisible rays are produced in the tube, traveling from the negati charged electrode (the cathode) to the positively charged electrode (the anod They produce glow on the zinc sulphide (a substance that produces a visible li when struck by a charged particle) coated glass wall of tube opposite to the catho These rays are emitted from cathode, hence called cathode rays.

Crookes and many other scientists conducted numerous experiments with discharge tubes to study the passage of electric discharge through gases during 1870s. From experiments, Crookes concluded that cathode rays were actually some sort of particles which possess momentum and kinetic energy, but other researches belived cathode rays were form of light.

In 1891, George Stoney, an Irish scientist, proposed that electricity was made of negatively charged particles called electrons.

(Electrons were first discovered by a British scientist, Joseph John Thomson (J.J. Thomson) in 1897, who was more interested in electricity than atomic structure. He modified Crookes tube and calculated the charge-to-mass ratio for the electron by studying the degree of deflections of cathode rays in different strengths of electric and magnetic fields. He concluded that electrons are much smaller and lighter than atoms. He found that the mass of one of these particles was almost 2,000 times lighter than a hydrogen atom. Thomson suggested that atoms were divisible, and that the electrons were the basic constituent of matter.

Joseph John Thomson
(1856-1940)

J. J. Thomson got Nobel Prize in 1906 in physics for discovery of electron and for his work on the conduction of electricity in gases.

Properties of Cathode Rays

i) In 1869, Hittorf observed that cathode rays produce shadow, when an opaque object is placed in their way. This proves that they travel in straight line in the absence of electrical and magnetic field.

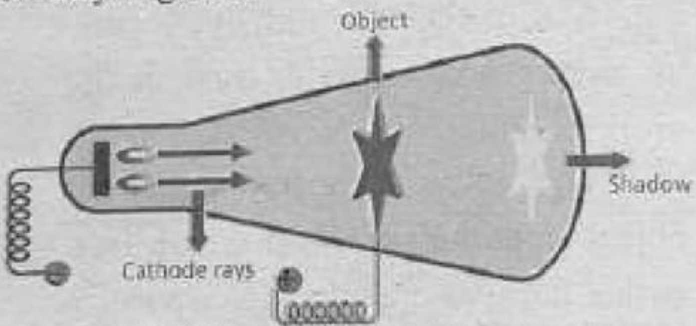

Figure 2.2: Cathode rays cast a shadow

ii) In 1870, William Crookes demonstrated that cathode rays can rotate a small thin mica paddle wheel placed in their way. It proves that cathode rays consist of particles having definite mass, velocity and momentum.

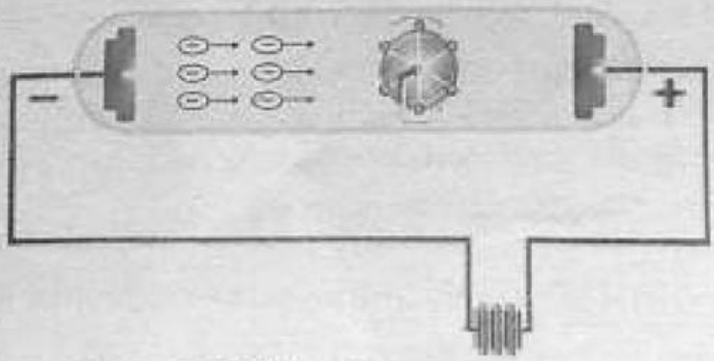

Figure 2.3: Cathode rays rotate a small paddle wheel

iii) In 1895, J. Perrin demonstrated that cathode rays bend towards positive plate of electric field. This shows that, they are negatively charged.

iv) In 1895, Wilhelm Roentgen demonstrated that cathode rays produce x-rays on striking with heavy metals anode like tungsten.

v) In 1897, J. J. Thomson demonstrated that if they are passed through magnetic field, the magnet neither attracts nor repels the particles but causes them to move in curved path perpendicular to the line drawn between the poles of the magnet.

vi) Thomson also determined e/m ratio of electrons. He found that the e/m value of electrons remained same, no matter which gas is used in the discharge tube.

vii) They increase the temperature of object (platinum foil) on which they strike. It proves that they have particle nature.

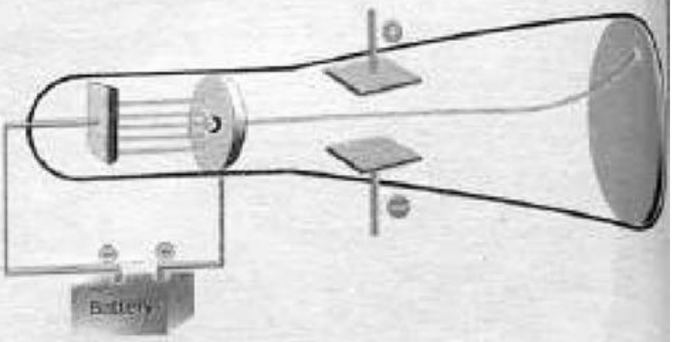

Figure 2.4: Deflection of cathode rays in the presence of electric field

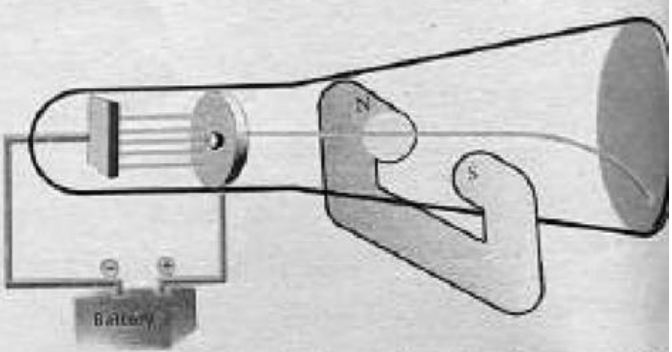

Figure 2.5: Deflection of cathode rays in the presence of magnetic field

Interesting Information

Nowadays cathode rays are used as advertisement neon signs. Television picture tube and monitors of computer are also cathode rays tube. The television and monitor pictures result due to fluorescence on the television and monitor screens coated with certain fluorescent materials.

viii) They produce glow when ZnS is placed in their way.

ix) They can ionize a gas.

x) They can pass through a very thin sheet of metal.

xi) They produce fogging effect on photographic plates.

xii) They can cause a chemical change because of their reducing power.

Measurement of e/m Ratio of Electron

In 1897, J. J. Thomson measured e/m ratio of electron. A discharge tube used for this purpose is shown here.

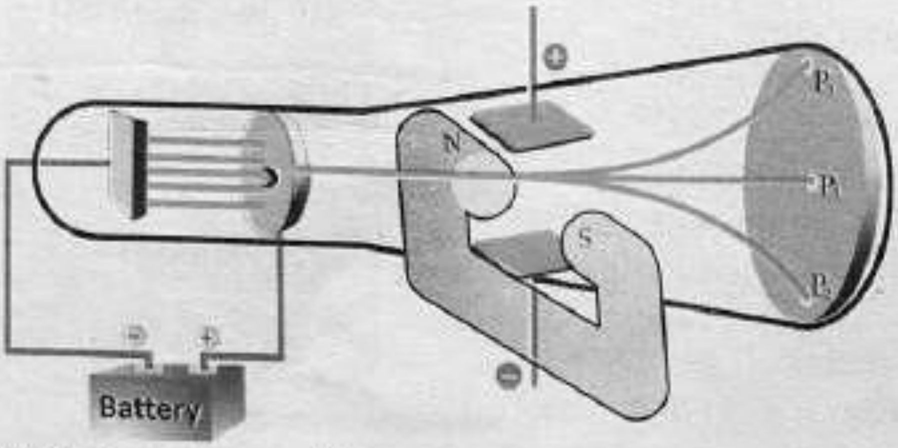

Figure 2.6: Discharge tube used for measurement of charge/mass ratio of an electron

In this experiment, a beam of cathode rays is passed through slits of anode. Then cathode rays (electrons) are allowed to pass through electric and magnetic fields. In the absence of any field, the beam of electrons gives bright luminous spot at P_1. When only magnetic field is applied, the beam of rays (electrons) strikes at point P_2. When only electric field is applied, the electrons strike at point P_3. When both the fields are applied simultaneously, then electrons again strike at point P_1. Hence by comparing the strengths of both the fields and with the help of mathematical calculations, J. J. Thomson determined the e/m ratio of electrons. Its calculated value is equal to 1.7588×10^{11} coulomb kg^{-1}, this means that 1kg of electrons have 1.7588×10^{11} coulombs charges.

After the charge-to-mass ratio for the electron had been determined, additional experiments were necessary to determine the value of its charge so that the mass should be calculated.

Robert Andrew Millikan (1868-1953)

Measurement of Charge on Electron (Millikan's Oil Drop Experiments)

In 1909, Robert Millikan working at the University of Chicago, determined the charge on electrons by oil drop experiment.

Construction

The apparatus consists of:

i) A metallic chamber having two parts:

(a) **The upper part:** It has an oil atomizer (sprayer).

(b) **The lower part:** It has two electrodes A and B. These electrodes are used to produce electric field in the space between the electrodes.

ii) There is a telescope in lower part to observe oil droplets.

iii) X-rays are used in the lower part of chamber for ionization of gas.

iv) An arc lamp is used to illuminate the space between the electrodes.

v) **A vacuum pump:** It is used to adjust the pressure inside the chamber.

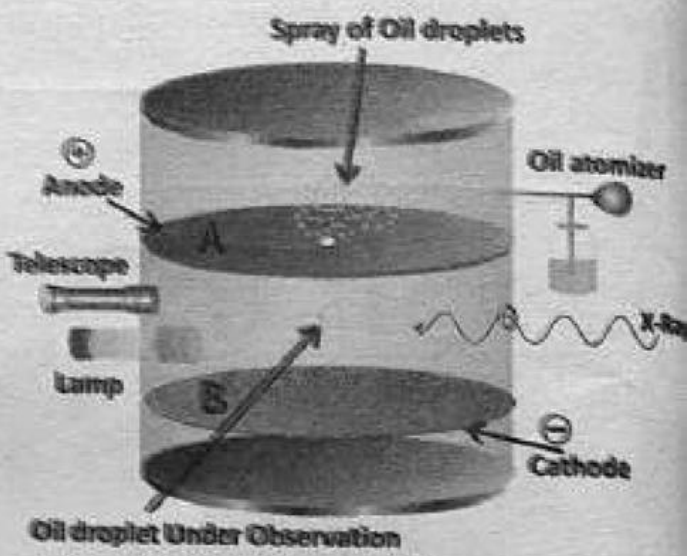

Figure 2.7: Millikan's oil drop experiment to measure the charge of an electron

Working

A fine spray of oil droplets is produced by atomizer in the space above the two plates (electrodes). A few drople enter the space between the two electrodes through the small hole. The hole closed at once; the arc lamp is turned on to illuminate the space between th electrodes. Without applying electric field, the droplet falls under the force gravity. The velocity of fall of the droplet is measured. The velocity of droplet directly proportional to its weight.

$$V_1 \propto mg \quad \text{..............} \quad (i)$$

Now the air present in the chamber is ionized by a beam of x-rays. In thi process, electrons are produced. The oil droplets take up electrons and becom charged. The electrodes A and B are then connected to a battery. In this way electric field is produced. Now droplet is under two forces (force of gravity an electric force). The charged droplets move up wards against the force of gravi with velocity V_2, when electric force is greater than that of gravitational force.

$$V_2 \propto H.e - mg \quad \text{..................} \quad (ii)$$

By dividing eq. (i) by (ii), we have:

$$\frac{V_1}{V_2} = \frac{mg}{H.e - mg} \quad \text{..................} \quad (iii)$$

By re-arranging eq. (iii), we have:

$$e = \frac{V_2 \times mg + mg}{V_1 \times H} \qquad \text{.......................(iv)}$$

By putting the values of velocities (V_1 and V_2), force of gravity (g), mass of droplet (m) and electric strength (H), the charge (e) on oil droplet is calculated.

By changing the strength of electric field (H), Millikan and his coworkers found that the charge on each droplet is different. The smallest charge which they found was 1.59×10^{-19} coulomb. This was the charge of one electron. This value is very close to the recent value of 1.602176×10^{-19} coulomb. With this value and the charge-to-mass ratio determined by Thomson, Millikan was able to calculate the mass of the electron as 9.11×10^{-31} kg.

Keep in Mind:

Millikan and his coworker measured hundreds of droplets and found that the charge on them was always a simple multiple of a basic unit, 1.59×10^{-19} coulomb. From this they concluded that the charge on an electron was numerically 1.59×10^{-19} coulomb.

Calculation of Mass of Electron

The mass of an electron can be calculated from the values of charge-to-mass ratio (e/m) and charge on electron (e).

e/m value of electron $= 1.758820 \times 10^{11}$ coulomb kg^{-1}

Charge of electron $= 1.602176 \times 10^{-19}$ coulomb / electron

Mass of an electron = ?

Mass of an electron $= \frac{e}{e/m}$

By putting the values, we have:

$$\text{Mass of electron} = \frac{1.602176 \times 10^{-19} C / \text{electron}}{1.758820 \times 10^{11} C/kg}$$

$$= 9.10938 \times 10^{-31} \text{kg/electron}$$

$$= 9.10938 \times 10^{-28} \text{g/electron}$$

.1.2 Discovery of Proton

n 1886, Eugen Goldstein took a discharge tube in which cathode was perforated. Ie observed that another type of rays was also travelling from anode to cathode long with cathode rays in the discharge tube. He observed a glow behind the athode. This was due to striking of rays on the glass wall after passing through the anals or holes of cathode. Hence these rays were passing through the canals of cathode; therefore, they were called canal rays. Later on these rays were called positive rays.

These rays do not emit from anode. They are positive ions which are formed due to striking of fast moving cathode rays (electrons) with gas molecules in the discharge tube. As a result of this, they eject electrons from the atoms of gas molecules.

Eugen Goldstein (1850-1930)

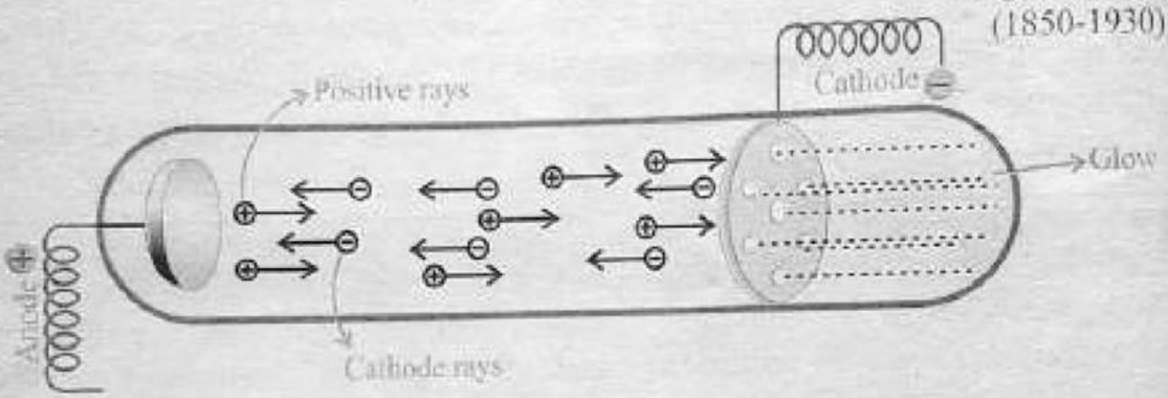

Figure 2.8: Canal rays

Properties of Canal Rays

Properties of canal rays are:

i) They move in straight line towards cathode.

ii) The behaviour of these particles in the magnetic or electrical field is opposite that observed for electron or cathode rays.

iii) Charge to mass (e/m) ratio is much smaller than that of electron. Charge to mass ratio depends upon the nature of gas present in the cathode rays tube. Heavier the gas, smaller the e/m ratio.

iv) The lightest and simplest positive ions (canal rays) were produced from hydrogen gas and were called protons. The name proton was given by Rutherford.

v) The mass of canal rays is never less than that of proton.

vi) Mass of proton (positive particle) is 1.00727amu or 1.6727×10^{-27} Kg.

vii) Charge of proton is 1.6022×10^{-19} coulombs.

Interesting Information:

The elements can be identified by the number of protons (atomic number) in their atoms. The atoms which have same number of protons are the atoms of the same element and the atoms which have different number of protons are the atoms of different elements.

2.1.3 Discovery of Neutron

In 1920, Rutherford predicted that some neutral particles having mass equal to proton must present in the nucleus of an atom. Because he observed that hydrogen atom has only one proton and that the helium atom has two protons. Therefore the mass of helium must be two times greater than that of hydrogen atom (electrons are much lighter than protons, their masses can be ignored). In reality, it was four times the mass of hydrogen atom. The added mass was due to another subatomic particle found in the nucleus, the neutron. But he failed to discover this sub atomic particle.

In 1932, a British scientist, Sir James Chadwick discovered neutron by artificial radioactivity and was awarded noble prize in Physics in 1935.

Sir James Chadwick
(1891-1974)

Chadwick bombarded a thin sheet of Beryllium by α-particles. He found that some highly penetrating radiations which have mass slightly greater than that of protons were produced. These radiations were called neutrons because the charge detector showed them to be neutral. Their nuclear reaction is:

$$^{4}_{2}He + ^{9}_{4}Be \longrightarrow ^{12}_{6}C + ^{1}_{0}n$$

Keep in mind:

- The neutron has about the same mass as the proton, but it has no electric charge. Any object that has no net electric charge is said to be electrically neutral, and that is where the neutron got its name.
- In a neutral atom the number of electrons is equal to the number of protons but the number of neutrons in a nucleus is not directly related to the numbers of protons and electrons.

Properties of Neutrons

Properties of neutrons are:

i) They are neutral particles.
ii) They cannot ionize gases.
iii) They are highly penetrating particles.
iv) They can knock protons out from paraffin, water, paper etc.
v) The mass of neutron is nearly equal to proton i.e. 1.00867 amu.
vi) Free neutron decays into a proton, electron and neutrino.

$$^{1}_{0}n \longrightarrow ^{1}_{+1}P + ^{0}_{-1}e + ^{0}_{0}n$$

vii) When neutrons travel with energy 1-20 MeV, they are called fast neutrons. When they travel with kinetic energy 1-10 eV, then they are called slow neutrons. Slow neutrons are more effective than fast neutrons.

viii) When they are used as a projectile, they can carry out nuclear reactions. For example:

a) $^{1}_{0}n + ^{14}_{7}N \longrightarrow ^{11}_{5}B + ^{4}_{2}He$

b) $^{1}_{0}n + ^{65}_{29}Cu \longrightarrow ^{66}_{29}Cu + h\nu$

$^{66}_{29}Cu \longrightarrow ^{66}_{30}Zn + ^{0}_{-1}e$

Uses:

They are used in the treatment of cancer, in nuclear fission and to produce radioactive elements.

Keep in mind:

The number of neutrons in the nuclei of atoms of the same element can be different. If two atoms have the same number of protons and different numbers of neutrons, they are atoms of the same element. However, they have different masses because of the different numbers of neutrons. Such atoms are said to be isotopes of each other. Each isotope of an element is usually identified by its mass number (A), which is defined as the sum of the number of protons and the number of neutrons in the nucleus of an atom.

Table 2.1: Properties of Three Fundamental Particles

Particle	Symbol	Charge in Coulomb	Mass in amu	Mass in grams	Relative Charge	Mass Relative to Electron
Electron	$^{0}_{0}e^{-}$	-1.6022×10^{-19}	0.00054	9.10938×10^{-28}	-1	-----
Proton	$^{1}_{1}P^{+}$	$+1.6022\times10^{-19}$	1.00727	1.67262×10^{-24}	$+1$	1836
Neutron	$^{1}_{0}n^{0}$	0	1.00867	1.67493×10^{-24}	0	1842

Example 2.1

How can you calculate the mass of proton relative to electron?

Solution:

Mass of proton $= 1.67262\times10^{-24}$ g

Mass of electron $= 9.10938\times10^{-28}$ g

Mass of proton relative to electron = ?

$$\text{Mass of proton relative to electron} = \frac{\text{Mass of proton}}{\text{Mass of electron}}$$

$$= \frac{1.67262 \times 10^{-24} g}{9.10938 \times 10^{-28} g}$$

$$= 1836$$

Practice Exercise 1:
How can you calculate the mass of neutron relative to electron?

2.2 Discovery of Nucleus and Rutherford's Atomic Model

2.2.1 Discovery of Nucleus

Rutherford
(1871 - 1937)

In 1911, the New Zealand physicist Lord Ernest Rutherford in England performed an experiment. He bombarded α-particles on thin gold foil of 0.00004cm. The α-particles were emitted from a radioactive metal (polonium or radium). During experiment, he observed that, most of the α-particles (more than 99%) passed through the metal foil directly without any deflection, but less than 1% (about 1 of every 20,000) was deflected at different angles. Some of these were deflected backward. They were detected by photographic plate coated by ZnS.

Results of this experiment were put forward by Rutherford in the form of Rutherford's Atomic Model.

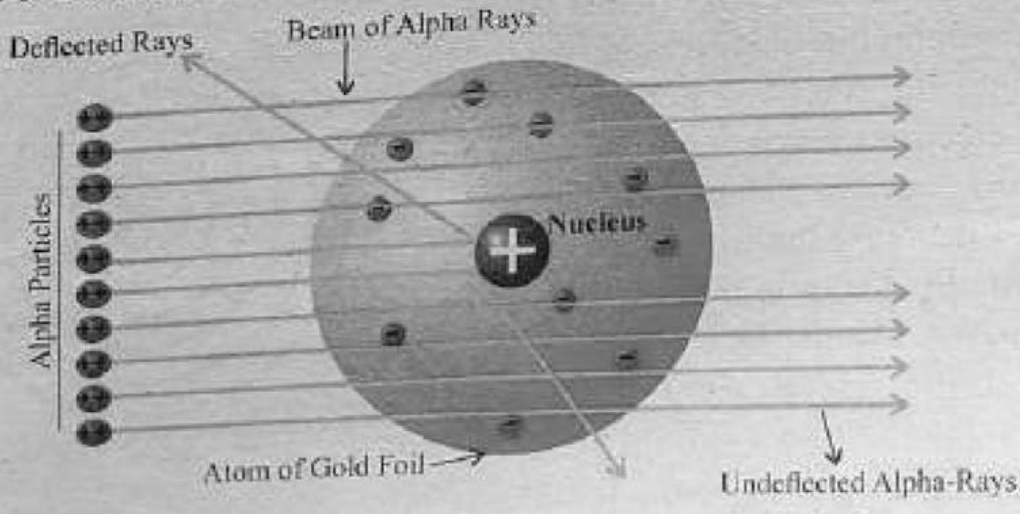

Figure 2.9: Few Alpha Rays are deflected which shows the presence of small positively charged nucleus

2.2.2. Rutherford's Atomic Model

Main points of Rutherford's atomic model are as follows:

i) Most of the volume of an atom is empty space in which electrons move around the nucleus.

ii) Nearly all the mass of an atom is present in the central part, called 'nucleus'.

iii) The size of nucleus is very small as compared to the size of atom.

iv) Nucleus of an atom has positive charge. This is indicated by wide range deflection of few-particles.

v) Positive charge on nucleus is equal the number of protons in the nucleus.

vi) The nucleus is surrounded by a number of negatively charged particles, called electrons.

vii) The number of electrons (negatively charged particles) is equal to number of protons (positively charged particles) in an atom. Therefore, atom as a whole is neutral.

viii) The electrons are in constant motion around the nucleus at large distances with very high velocities like plants around the sun in their orbits.

ix) Protons and neutrons are present in the nucleus and they are called nucleons.

x) There is electrostatic force of attraction between protons and electrons.

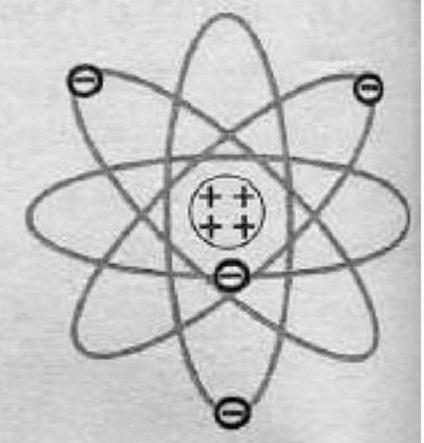

Figure 2.10: Rutherford's Atomic Model

Defects in Rutherford's Model

Rutherford's atomic model was similar to our solar system. It has following defects:

i) Rutherford's atomic model was based on the laws of gravitation and motion which could applied to the neutral bodies like plants but not to the charged particles like electrons and protons.

ii) According to Maxwell's theory, charge particles i.e. electrons revolving in an orbit must radiate (emit) energy. Therefore energy of electron must decrease and it will go into spiral motion. So finally it should fall into the nucleus. Thus the atom would collapse.

iii) If revolving electrons release energy continuously, then they should produce a continuous spectrum but in actual practice, line spectrum in produced by an atom.

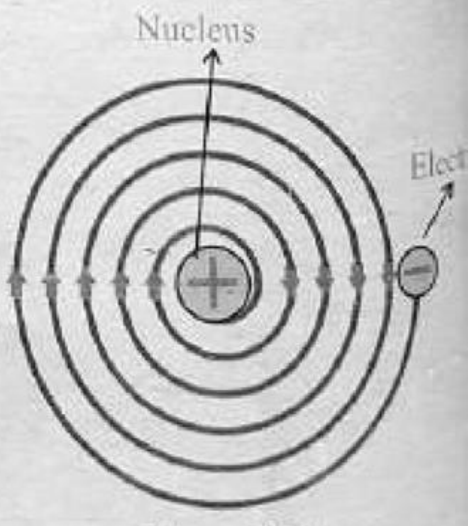

Figure 2.11: Spiral Motion of Electron

2.3 Planck's Quantum Theory

Max Planck
(1858–1947)

In 1900, a German physicist Max Planck gave quantum theory of radiation. He studied the emission and absorption of radiations which are obtained from hot objects at different temperatures. Planck said that atoms and molecules could emit or absorb energy only in discrete quantities (small bundles). Planck gave the name quantum (meaning "fixed amount") to the smallest quantity of energy that can be emitted or absorbed in the form of electromagnetic radiations.

Main points of this theory are:

i) Energy is not emitted or absorbed continuously in radiation form.

ii) Energy is emitted or absorbed in packets. Each packet is called quantum. In case of light, the wave packets are often called photon.

iii) Energy of each quantum is directly proportional to the frequency of radiation.

$E \propto \nu$ or

$E = h\nu$ .... (i)

Where, E is Energy of quantum, ν (nu) is Frequency and h is Planck's constant. Its value is 6.6262×10^{-34} J. sec.

iv) An atom or molecule can emit or absorb either quantum of energy ($h\nu$) or any integral multiple of a quantum ($nh\nu$)

$E = nh\nu$ .... (ii)

Where, $n = 1, 2, 3, 4, ... \infty$

The energy can be emitted as $h\nu$, $2h\nu$, $3h\nu$ and so forth but never as $1.5h\nu$, $2.6h\nu$, $4.3h\nu$ or any other fractional value of $h\nu$.

In 1918 Planck was awarded the Nobel Prize in Physics for his work on the quantum theory.

Frequency

The number of waves passing through a point in one second is called frequency. It is shown by ν. Its units are hertz or cycles/sec. It is measured by spectrometer.

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

Where c is velocity of light that is 3×10^8 m/sec and λ (Lambda) is wavelength.

Note that ν is directly proportional to c and inversely proportional to λ.

Wavelength

The distance between two adjacent crests or troughs of wave is called wavelength. It is shown by λ (Lambda). Its units are m, nm or A°.

Table 2.2: Units of Wavelength for Electromagnetic Radiations

Unit	Symbol	Wavelength(m)	Radiation Type
Meter	M	1	Radio waves
Centimeter	cm	10^{-2}	Microwave
Millimeter	mm	10^{-3}	Infrared
Micrometer	µm	10^{-6}	Infrared
Nanometer	nm	10^{-9}	Ultraviolet, Visible
Angstrom	A°	10^{-10}	X-ray
Picometer	pm	10^{-12}	Gamma ray, Cosmic ray

Amplitude

The vertical distance from the midline of a wave to the crest or trough is called amplitude.

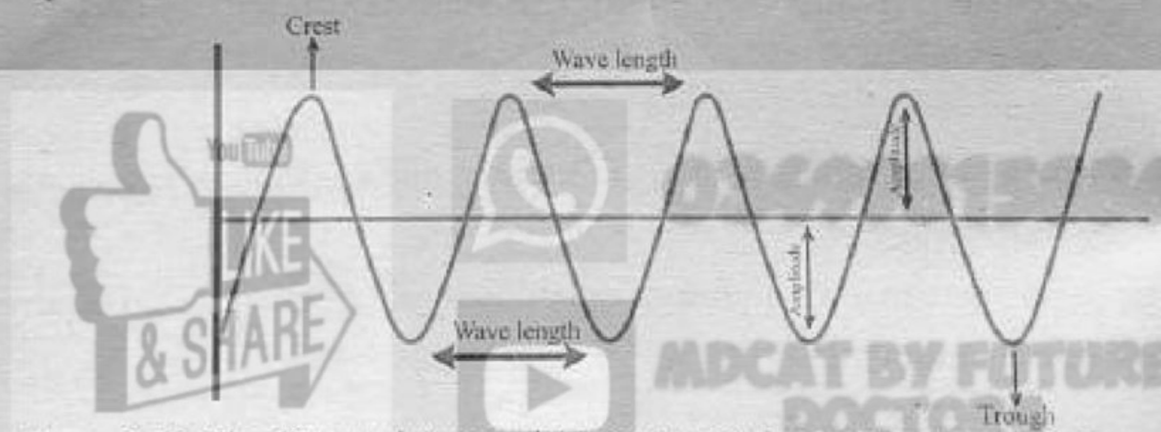

Figure 2.12: The distance between the two consecutive crest or trough is the wavelength and the height of the wave from the midline is the amplitude

Wavenumber

The number of waves present in one centimeter distance is called wave number. It is the inverse of wave length. It is shown by $\bar{\nu}$ (nu bar).

As,

$$\nu = c\bar{\nu}$$

Hence,

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

Its unit is cm^{-1}. Its SI unit is m^{-1}.

Atomic Number

The number of protons in an atom is called atomic number. It is also called proton number. It is shown by Z. Atoms are neutral because they have the same number electrons and protons. The number of electrons in a neutral atom is also equal to the atomic number.

Relation between Frequency and Wavelength

The frequency is related to the wavelength of the photon as:

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

By putting the value of v in equation (i), we get

$$E = h.\frac{c}{\lambda} \qquad \text{.............................} \quad \text{(iii)}$$

So, energy of photon is directly proportional to velocity of light and inversely proportional to wavelength.

Relation between Wavelength and Wavenumber

Wave number ($\bar{\nu}$) is the inverse of wavelength.

$$\bar{\nu} = \frac{1}{\lambda} \qquad \text{or}$$

$$E = hc\bar{\nu} \qquad \text{.............................} \quad \text{(iv)}$$

So, energy of photon is directly proportional to wave number.

2.4 Bohr's Atomic Model

In 1913, the Danish scientist Neil Henrik David Bohr explained spectrum of hydrogen atom. He received the Noble Prize in Physics in 1922 for this work. Bohr's theory was based on Planck's quantum theory.


Neil Henrik David Bohr (1885–1962)

The main points of this theory are:

i) Electrons revolve around the nucleus in the circular path called orbits or energy levels or shells. Electrons in each orbit have a definite amount of energy and are at a fixed distance from the nucleus.

ii) Electron does not radiate (emit or absorb) energy as long as it is revolving in its orbit.

iii) The electron absorbs energy when it jumps from lower orbit to higher orbit and it loses energy of one photon when it jumps from higher to lower orbit.

iv) When an electron jumps from one orbit to another orbit, there will be a change in energy. For example when an electron jumps from first orbit (E_1) to second orbit (E_2), then the energy change is given by Planck's equation,

$E_2 - E_1 = h\nu$ or

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

Where,

ΔE is change in energy, 'h' is Planck's constant and 'ν' is frequency

The angular momentum (mvr) of an electron revolving around the nucleus is quantized. It is an integral multiple of Planck's constant (nh) divided by 2π.

$$\text{Angular momentum (mvr)} = \frac{nh}{2\pi}$$

Where,

n = 1, 2, 3, 4, ... ∞. It represents number of orbits.

'm' is mass of electron, 'v' is velocity of electron and 'r' is radius of orbit.

By putting the values 1, 2, 3, etc. of n, we have:

$$\frac{h}{2\pi}, \frac{2h}{2\pi}, \frac{3h}{3\pi}, \text{ etc.}$$

There is no fractional value for $\frac{nh}{2\pi}$.

An atom has only a limited number of permitted energy levels, and an electron is bound to remain in one of these energy levels (orbits) and not in between them. This is analogous to steps on a staircase. Where you are on a staircase is bound to stand on any one of the steps and you cannot stand between two adjacent steps.

2.4.1 Derivation of Radius, Energy, Frequency, Wavelength, and Wavenumber:

Calculation of Radius of Orbit

Consider an electron of charge *e* and mass *m* is revolving around the nucleus with velocity v at a distance r. Nucleus has total charge Ze^+, where Z is the proton number and e^+ is the charge on proton. There are two forces acting on electron:

i) The attractive or centripetal force

ii) The repulsive or centrifugal force.

The centrifugal force which takes electron away from nucleus is:

$$F = \frac{mv^2}{r} \quad \text{.................... (i)}$$

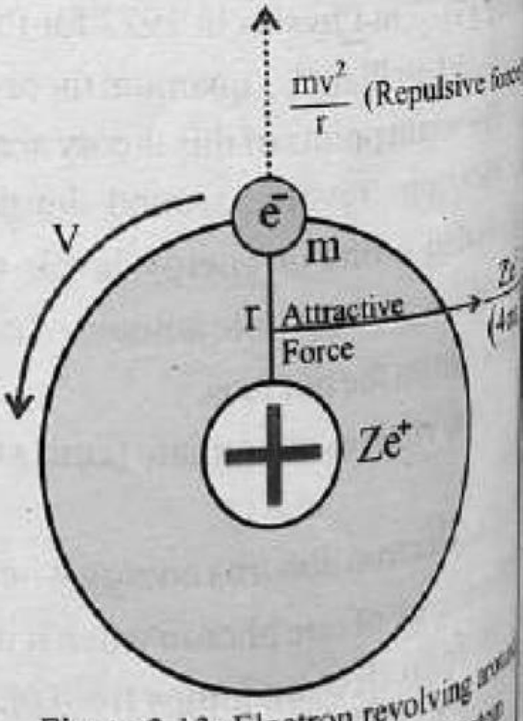

Figure 2.13: Electron revolving around the nucleus in the hydrogen atom

The electrostatic force of attraction (centripetal force) between electron and nucleus is:

$$F \propto \frac{Ze.e}{r^2} \qquad \text{or}$$

$$F \propto \frac{Ze^2}{r^2} \qquad \text{or}$$

$$F = \frac{Ze^2}{(4\pi\varepsilon_o)r^2} \qquad \text{.................... (ii)}$$

Where, $4\pi\varepsilon_o$ is proportionality constant. ε_o (Epsilon not) is vacuum permittivity. Its value is equal to $8.8545\times10^{-12}\,C^2J^{-1}m^{-1}$.

In order to keep the electron in its orbit, the centrifugal force must be equal to centripetal force.

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\varepsilon_o r^2}$$

$$v^2 = \frac{Ze^2 r}{4\pi\varepsilon_o r^2 m}$$

$$v^2 = \frac{Ze^2}{4\pi\varepsilon_o rm} \qquad \text{...................... (iii)}$$

According to Bohr's atomic model, the angular momentum of an electron is:

$$mvr = \frac{nh}{2\pi} \qquad \text{or}$$

$$v = \frac{nh}{2\pi mr}$$

By taking the square, we have:

$$v^2 = \frac{n^2h^2}{4\pi^2m^2r^2} \qquad \text{...................... (iv)}$$

By putting the value of v^2 from eq. (iv) in eq. (iii), we get

$$\frac{Ze^2}{4\pi\varepsilon_o r\,m} = \frac{n^2h^2}{4\pi^2m^2r^2}$$

Now, we can calculate the value of r,

$$\frac{r^2}{r} = \frac{n^2h^2}{4\pi^2m^2} \times \frac{4\pi\varepsilon_o m}{Ze^2}$$

$$r = \frac{n^2h^2\varepsilon_0}{\pi mZe^2} \quad \text{.............................} \quad (v)$$

Equation (v) can be written as,

$$r = \frac{h^2\varepsilon_0}{\pi me^2} \times \frac{n^2}{Z}$$

This equation tells us that, the radius, r of an atom is directly proportional to the square of number of orbit (n). So higher orbit has larger radius. In the eq. (v), the factor $\frac{h^2\varepsilon_0}{\pi me^2}$ is constant. Its value is 0.529A° (52.9pm or 5.29×10^{-10}m). It is denoted by a_0 (Bohr's radius).

Hence,

$$a_0 = \frac{h^2\varepsilon_0}{\pi me^2}$$

Therefore,

$$\boxed{r = \frac{n^2}{Z} \times a^0} \quad \text{or}$$

$$r \propto \frac{n^2}{Z}$$

The above relationship shows that,

i) The radius of an atom is directly proportional to the square of number of orbits.

ii) The radius (r) of an atom is inversely proportional to the atomic number (number of proton) Z.

Example 2.2

Calculate the radius of first four orbits of electron of hydrogen atom.

Solution:

The equation to calculate the radius of an orbit is:

$$r = \frac{n^2}{Z} \times a_0$$

The atomic number (Z) of hydrogen atom = 1

Bohr's radius (Value of a_0) = 0.529A°

By putting the values of n as 1, 2, 3, 4 in the equation we get:

Radius of first orbit of hydrogen atom $(r_1) = \frac{(1)^2}{1} \times 0.529\mathring{A} = 0.529\mathring{A}$

Radius of second orbit of hydrogen atom $(r_2) = \frac{(2)^2}{1} \times 0.529\mathring{A} = 2.11\mathring{A}$

Radius of third orbit of hydrogen atom $(r_3) = \frac{(3)^2}{1} \times 0.529\mathring{A} = 4.75\mathring{A}$

Radius of fourth orbit of hydrogen atom $(r_4) = \frac{(4)^2}{1} \times 0.529\mathring{A} = 8.46\mathring{A}$

It is cleared from the above data that distance between orbits goes on increasing from lower to higher orbits. Hence,

$r_2 - r_1 < r_3 - r_2 < r_4 - r_3 < \ldots$

i) The second orbit is four times away from the nucleus than that of first orbit.

ii) The third orbit is nine times away and fourth orbit is sixteen times away from the nucleus.

Calculation of Energy of an Electron (in H-atom)

Total energy of an electron revolving around the nucleus is the sum of its kinetic and potential energies.

$$E = K.E + P.E \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (vi)$$

$$K.E = \frac{1}{2} mv^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (vii)$$

Potential energy is the amount of total work done for bringing the electron from infinity to distance r.

$$P.E = -\frac{Ze^2}{4\pi\varepsilon_o r} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (viii)$$

In equation (viii) minus sign shows that the energy is released (or decreased) due to attraction between electron and nucleus.

By putting the values of equation (vii) and (viii) in equation (vi), we have

$$E = \left(\frac{1}{2} mv^2\right) + \left(-\frac{Ze^2}{4\pi\varepsilon_o r}\right)$$

$$E = \frac{1}{2} mv^2 - \frac{Ze^2}{4\pi\varepsilon_o r} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (ix)$$

By putting the value of v^2 from equation (iii) in equation (ix), we have

$$E = \frac{1}{2} m.\frac{Ze^2}{4\pi\varepsilon_o r m} - \frac{Ze^2}{4\pi\varepsilon_o r} \qquad \text{or}$$

$$\because v^2 = \frac{Ze^2}{4\pi\varepsilon_o rm}$$

$$E = \frac{Ze^2}{8\pi\varepsilon_o r} - \frac{Ze^2}{4\pi\varepsilon_o r}$$

By taking LCM we have,

$$E = \frac{Ze^2 - 2Ze^2}{8\pi\varepsilon_o r}$$

$$E = -\frac{Ze^2}{8\pi\varepsilon_o r} \qquad \text{..........................(x)}$$

By putting the value of *r* in equation (x), we have

$$E = -\frac{Ze^2}{8\pi\varepsilon_o \frac{n^2h^2\varepsilon_o}{\pi mZe^2}} \qquad \text{or}$$

$$\because r = \frac{n^2h^2\varepsilon_o}{\pi mZe^2}$$

$$E = -\frac{Ze^2}{8\pi\varepsilon_o} \times \frac{\pi mZe^2}{n^2h^2\varepsilon_o} \qquad \text{or}$$

$$E = -\frac{Z^2e^4m}{8\varepsilon_o^2n^2h^2} \qquad \text{or}$$

$$E = -\frac{e^4m}{8\varepsilon_o^2h^2} \times \frac{Z^2}{n^2} \qquad \text{..........................(xi)}$$

In the above equation when constants (8, e, m, ε_o, h) are replaced by constant K, the equation (xi) will become:

$$E = -K \times \frac{Z^2}{n^2}$$

$$\because \frac{e^4m}{8\varepsilon_o^2h^2} = K$$

Energy of electron in the nth orbit is:

$$E_n = -K \times \frac{Z^2}{n^2}$$

The value of K is 2.18×10^{-18}J, hence the equation can be written as:

$$E_n = -2.18\times10^{-18}\,J \times \frac{Z^2}{n^2} \qquad \text{..........................(xii)}$$

Where,

E_n = energy of the electron in the nth orbit.

Z = Atomic number of the element.

n = Principal quantum number. It shows number of shells.

In the above equation:

i) The negative sign shows that the electron is bound to the nucleus in the orbit by the electrostatic force of attraction.

ii) As the value of *n* increases, the value of *E* should decrease but due to presence of negative sign in the formula, the actual value of energy will increase.

Example 2.3

Calculate the energies of electron of first four shells (orbits) of hydrogen atom.

Solution:

The equation to calculate the energy of electron in a shell is:

$$E_n = -2.18 \times 10^{-18}\ J \times \frac{Z^2}{n^2}$$

Atomic number of Hydrogen = Z = 1

Energy of electron in the 1^{st} orbit (n = 1) = $E_1 = -2.18 \times 10^{-18}\ J \times \frac{(1)^2}{(1)^2}$

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

Energy of electron in the 2^{nd} orbit (n = 2) = $E_2 = -2.18 \times 10^{-18} J \times \frac{(1)^2}{(2)^2}$

$= -0.54 \times 10^{-18} J$

Energy of electron in the 3^{rd} orbit (n = 3) = $E_3 = -2.18 \times 10^{-18} J \times \frac{(1)^2}{(3)^2}$

$= -0.24 \times 10^{-18} J$

Energy of electron in the 4^{th} orbit (n = 4) = $E_4 = -2.18 \times 10^{-18} J \times \frac{(1)^2}{(4)^2}$

$= -0.14 \times 10^{-18} J$

We can see that energy of the electron increases when number of orbits increases.

$$E_1 < E_2 < E_3 < E_4$$

Calculation of Energy Difference (ΔE):

ΔE is the amount of energy released or absorbed when an electron jumps from one orbit to another orbit.

$$\Delta E = E_2 - E_1 \qquad \text{.....................} \quad \text{(xiii)}$$

According to Bohr's equation, the energy of electron in an orbit is:

$$E_n = -K \times \frac{Z^2}{n^2}$$

The energy of electron in any lower orbit (n_1) is:

$$E_1 = -K \times \frac{Z^2}{n_1^2}$$

The energy of electron in any higher orbit (n_2) is:

$$E_2 = -K \times \frac{Z^2}{n_2^2}$$

By putting the values of E_1 and E_2 in equation (xiii) we have:

$$\Delta E = (-K \times \frac{Z^2}{n_2^2}) - (-K \times \frac{Z^2}{n_1^2}) \quad \text{or}$$

$$\Delta E = (-K \times \frac{Z^2}{n_2^2} + K \times \frac{Z^2}{n_1^2}) \quad \text{or}$$

$$\Delta E = K \times \frac{Z^2}{n_1^2} - K \times \frac{Z^2}{n_2^2} \quad \text{or}$$

$$\Delta E = KZ^2[\frac{1}{n_1^2} - \frac{1}{n_2^2}] \qquad \text{.....................} \quad \text{(xiv)}$$

For Hydrogen atom $Z = 1$, hence,

$$\Delta E = K[\frac{1}{n_1^2} - \frac{1}{n_2^2}]$$

We know that the value of $K = 2.8 \times 10^{-18}$ J, therefore,

$$\Delta E = 2.18 \times 10^{-18} \text{ J}[\frac{1}{n_1^2} - \frac{1}{n_2^2}]$$

Example 2.4

Calculate the amount of energy needed when an electron jumps from second orbit ($n = 2$) to fourth orbit ($n = 4$) of hydrogen atom.

Solution:

Amount of energy needed = ΔE = ?

The value of constant K = 2.18×10^{-18}J

The equation to calculate the ΔE is:

$$\Delta E = 2.18\times10^{-18}\,J[\frac{1}{n_1^2}-\frac{1}{n_2^2}]$$

By putting the values we have,

$$\Delta E = 2.18\times10^{-18}\,J[\frac{1}{(2)^2}-\frac{1}{(4)^2}]$$

$$= 2.18\times10^{-18}\,J[\frac{1}{4}-\frac{1}{16}]$$

$$= 2.18\times10^{-18}J\,[\frac{4-1}{16}]$$

$$= 2.18\times10^{-18}J[\frac{3}{16}]$$

$$= 2.18\times10^{-18}J\times0.1875$$

$$= 4.087\times10^{-19}J$$

Calculation of Frequency

According to Planck's theory, the energy change (ΔE) is directly proportional to the frequency of radiation.

$$\Delta E = h\nu$$

We know that,

$$\Delta E = KZ^2[\frac{1}{n_1^2}-\frac{1}{n_2^2}]$$

Therefore,

$$h\nu = KZ^2[\frac{1}{n_1^2}-\frac{1}{n_2^2}] \quad \text{or}$$

$$\nu = \frac{KZ^2}{h}[\frac{1}{n_1^2}-\frac{1}{n_2^2}] \quad \text{.............................} \quad \text{(xv)}$$

Unit of frequency is cycles per second or Hertz.

Calculation of Wave number

We know from Planck's theory that,

$$\nu = c\bar{\nu}$$

We also know that,

$$\nu = \frac{KZ^2}{h}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

By putting the value of ν in the above equation, we get,

$$c\bar{\nu} = \frac{KZ^2}{h}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\bar{\nu} = \frac{KZ^2}{hc}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \qquad \text{or}$$

$$\bar{\nu} = \frac{K}{hc}.Z^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

The constants $\frac{K}{hc}$ can be replaced by constant R_∞ (Rydberg's constant) as

$$\bar{\nu} = R_\infty Z^2\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

For hydrogen atom Z=1, therefore,

$$\bar{\nu} = R_\infty\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

Unit of wave number is m^{-1}.

The value of R_∞ is $1.09678 \times 10^7 m^{-1}$.

Usefulness of Bohr's Atomic Model

i) It is useful to calculate the radius of an orbit.
ii) It is useful to calculate the energy of an electron.
iii) It helped to calculate the ΔE, frequency and wavenumber.
iv) It explained the spectra of hydrogen and hydrogen like atoms (ions) such He^{1+}, Li^{2+} and Be^{3+}.
v) It explained the stability of atoms and their ionization energy.
vi) It shows the orbits in hydrogen atom.

2.4.2 Spectrum of Hydrogen Atom

Hydrogen spectrum is an important example of atomic spectrum. When hydrogen gas is filled in discharge tube at very low pressure and then high voltage is applied bluish light is emitted from discharge tube. If this light is passed through spectrometer, several sharp lines of different wavelengths are produced. They are called spectral lines. These spectral lines are classified into five groups called spectral series. These series were named after their discoverers.

i) Lyman Series ii) Balmer Series
iii) Paschen Series iv) Bracket Series
v) Pfund Series

The first four series were discovered before Bohr's atomic model.

Origin of Hydrogen Spectrum

We know that, there is one electron in hydrogen atom which is present in first orbit at room temperature. This is the lowest energy state or ground state of this electron. When hydrogen gas is heated, its electron jumps from lower energy state i.e. $n_1 = 1$ to higher energy state or excited state i.e. $n_2 = 2, 3, 4, 5, 6, 7$ etc. depending upon the amount of energy absorbed. Now the electron will become unstable. When it comes back from higher energy levels i.e. $n_2 = 2, 3, 4, 5, 6, 7$ etc. to lower energy level i.e. $n_1 = 1$, the same amount of energy is released in the form of spectral lines (bright lines). The series of spectral lines are as follows:

Lyman Series

When an electron jumps from a higher energy level n_2(i.e. 2, 3, 4, 5, 6 etc.) to lower energy level n_1 (i.e. 1), a series of spectral lines are produced. This series of lines appears in the UV region of the spectrum.

Balmer Series:

When an electron jumps from a higher energy level n_2(i.e. 3, 4, 5, 6 etc.) to a lower energy level n_1 (i.e. 2), a series of spectral lines are produced. This series appears in the visible region.

Paschen Series:

When an electron jumps from a higher energy level n_2 (i.e. 4, 5, 6, etc.) to a lower energy level n_1 (i.e. 3), a series of spectral lines are produced. This series appears in the infra-red region.

Bracket Series:

When an electron jumps from a higher energy level n_2 (i.e. 5, 6, etc.) to a lower energy level n_1 (i.e. 4), a series of spectral lines are produced. This series appears in infra-red region.

Pfund Series:

When an electron jumps from a higher energy level n_2 (i.e. 6, 7, etc.) to a lower energy level n_1 (i.e. 5), a series of spectral lines are produced, called pfund se[ries]. This series appears in infra-red region.

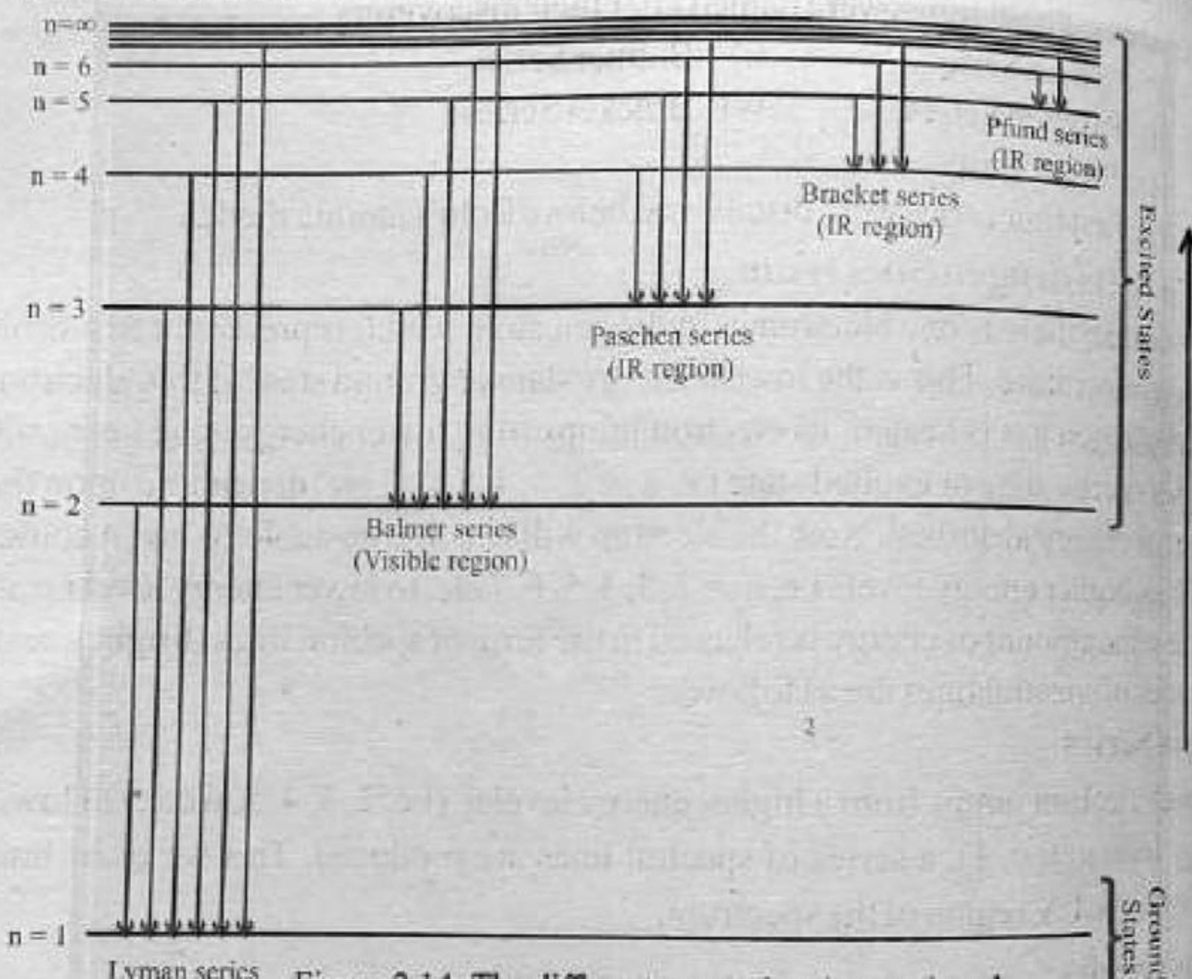

Figure 2.14: The different spectral series produced due to electronic transitions

Table 2.3: The Series of Spectral Lines

Series of Spectral Lines	Jumping of Electrons		Region	Wavelength (A°)
	n_2	n_1		
Lyman	2, 3, 4, 5 ... ∞	1	Ultraviolet	920 – 1200
Balmer	3, 4, 5, 6 ... ∞	2	Visible	400 – 6500
Paschen	4, 5, 6, 7 ... ∞	3	Infra-red	9500 – 18750
Bracket	5, 6, 7, 8 ... ∞	4	Infra-red	19450 – 40500
Pfund	6, 7, 8, 9 ... ∞	5	Infra-red	38000 – 75000

2.4.3 Defects of Bohr's Atomic Model

It failed to explain:

i) The spectrum of more complicated (multi electron) atoms.
ii) The objections raised on Rutherford's atomic model.
iii) Zeeman Effect (splitting of spectral lines into still thinner and closely spa[ced]

lines in the presence of magnetic field) and Stark effect (splitting of spectral lines into still thinner and closely spaced lines in the presence of electric field).

iv) Motion of electrons in three dimensional spaces. It explains motion of electrons in circular orbits.

Reason of Zeeman and Stark Effects

When a strong electric and magnetic field is applied, the spectral line of sodium atom splits up into further thinner closely spaced lines. The number of closely spaced lines is corresponding to the number of values of magnetic quantum number. Hence each line represents an orbital.

Society, Technology and Science

Firework Displays:

Firework is a device containing explosives and combustible chemicals that generate coloured lights, smoke and noise and are used for display and celebrations. There is a lot of chemistry involved in fireworks. The colours that appear in fireworks are due to the presence of different metal compounds. The metal compounds emit characteristic colours when heated. When an element is heated, its electron jumps from lower energy state (ground state) to higher energy state (excited state). Now the electron will become unstable. When it comes back from higher energy state to lower energy state, the energy is released as light of specific colours. The colour of light depends on the element (metal) to be heated. For example, lithium compounds ($LiCO_3$) create **red** colours; sodium compounds (NaCl) create **yellow** colours, barium compounds ($BaCl_2$) create **green** colours, copper compounds ($CuCl_2$) create **blue-green** colours, potassium compounds (KNO_3) create **violet-pink** colours, rubidium compounds ($RbNO_3$) create **violet-red** colours, and aluminum, beryllium or magnesium powders create bright white colours in fireworks.

2.5 X-Rays

2.5.1 Production, Properties and Uses

Production of X-Rays

Wilhelm Conrad Roentgen (1845-1923)

In 1895, a German Scientist Wilhelm Conrad Roentgen discovered that when fast moving electrons collide with heavy metal anode in the discharge tube, some unknown very high energy rays are produced. They were called X-rays. X-rays are electromagnetic radiations. They are not visible and are of higher frequency and shorter wavelength than visible light. Roentgen was awarded the Nobel Prize in 1901

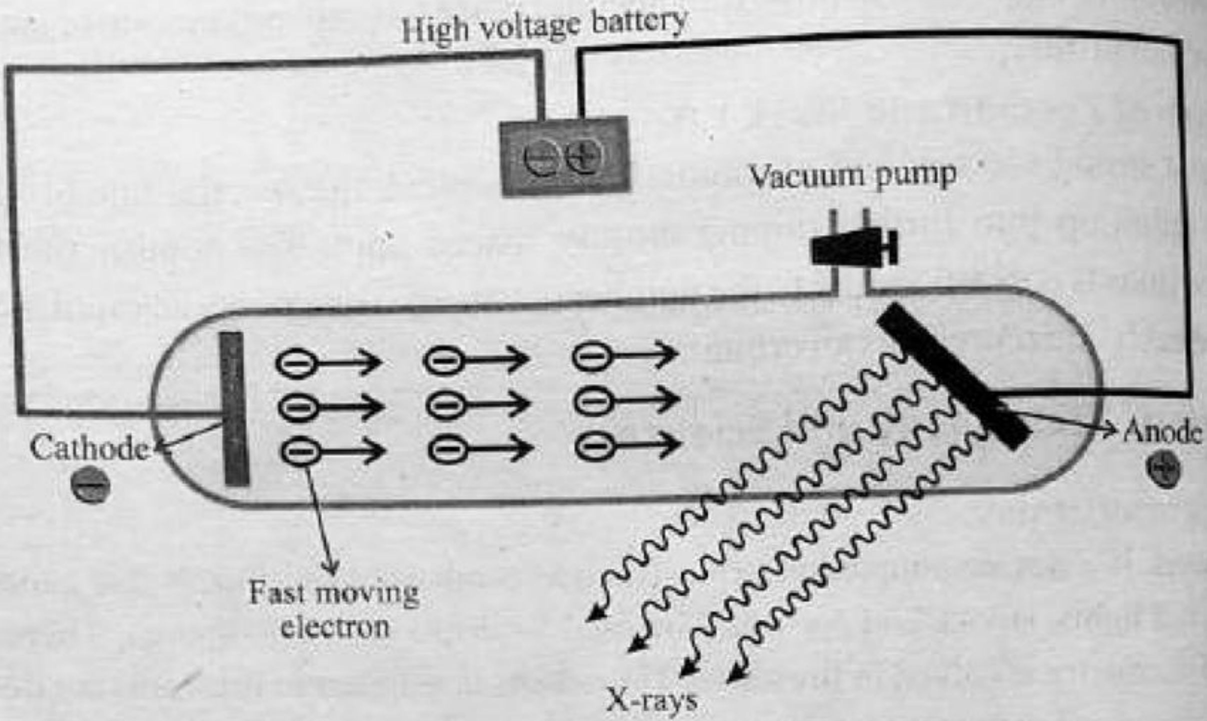

Figure 2.15: Production of X-rays

Properties of X-Rays

i) They are electromagnetic radiations and cannot be deflected by electric and magnetic fields. Thus, travel in straight lines.

ii) They are invisible to the eyes but can affect the photographic plate.

iii) They have very high penetrating power through matter. This is because the rays are used to study the interior of the objects.

iv) They can damage genes, chromosomes and other cell components when passing through living tissues.

v) They are highly energetic rays. Therefore, they ionize gases.

vi) They have high frequency. Their frequency depends upon the material anode. Due to this reason, different elements produce X-rays of different wavelengths.

vii) The frequency of X-rays increases with atomic number of the element used anode in the X-rays tube.

viii) Frequency of X-rays ranges from 3×10^{16} to 3×10^{19}Hz.

ix) The wavelength of X-rays range from 0.01 to 10nm.

Keep in Mind:

- Electromagnetic radiation is a form of energy that travels through space at a constant speed of $3\times10^8 ms^{-1}$ and can exhibit wavelike or particle-like properties.
- The wavelength of electromagnetic radiation determines the amount of energy carried by one of its photons. The shorter the wavelength, the greater the energy of each photon.
- The frequency and energy of electromagnetic radiations are inversely proportional to its wavelength.

Uses of X-Rays

i) X-rays diffraction techniques are used in the study of crystal structure because X-ray wave lengths are comparable to the atomic separation distances in solids (about 0.1nm).

ii) X-rays are used as a diagnostic tool in medicine and as a treatment for certain forms of cancer.

iii) X-ray images are used for the detection of dental cavities, bone fractures and to differentiate between hard tissues (bone) and soft tissues (blood and muscles). X-rays pass through soft body tissue but are stopped by harder tissue.

iv) When high energy X-ray photons are passed through gases, they increase the temperature of atoms and molecules and electrons are ejected. These free electrons may ionize additional neutral species. Through this process, reactive ions and free radicals are formed, leading to further chemical reactions.

v) X-rays are used for quick examination to check the luggage of passengers at air ports.

vi) In industry, X-ray images are used to detect flaws (i.e. cracks) non-destructively in metal castings that are invisible.

vii) X-ray microscopes are capable of magnifying X-ray absorption images so as to resolve features on scales as small as about 40nm.

viii) The presence of coatings and varnishes, and the compositions of glasses, porcelain, and enamels are revealed through X-ray analysis.

ix) X-rays are used to study chemical reactions on surfaces, the electronic structures of semiconductors and magnetic materials, and the structure and function of proteins and biological macromolecules.

2.5.2 Types of X-Rays

When an electron in the cathode rays collides with metal anode (target), it can kno an electron from an inner shell (K-shell) of the atom. The knocked electron w have to leave the atom because there is no vacancy in the higher energy levels. Th produces a vacancy (hole) in the inner shell. The electron from high energy levels (i.e. L-shell or M-shell) then drops down to fill the vacancy, emitting a high energy photon of X-rays. L-shell to K-shell jump produces a K_{α} X-ray. M-shell to K-shell jump produces a K_{β} X-ray. The energy of the K_{β} transitions is higher than that of the K_{α} transitions.

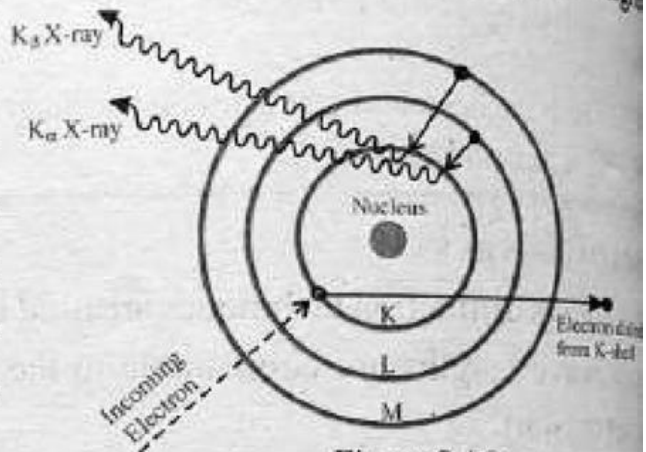

Figure 2.16: Types of X-rays

2.6 Quantum Numbers and Orbitals

After the failure of Bohr's atomic model, in 1926, an Austrian Physicist Erw Schrodinger, an expert on the theory of vibrations and standing waves, set up a wa equation for hydrogen atom. This is called Quantum Mechanical Model of an ato Schrodinger was awarded noble prize in Physics in 1933 for setting up t equation. The main problem before Schrodinger was where we would find t electron if we were to look for it. According to Schrodinger:

Erwin Schroding (1887–1961)

Although the position of an electron cannot be found exactly, the probability of finding the electron at a particular position in space can be found.

The concept of electron density gives the probability that an electron will be found in a particular region of an atom. The most likely place to find an electron is where the density is greatest. An atomic orbital is the wave function of an electron in an atom. The wave function and its square, ψ^2 (Psi) have values fo locations about a nucleus. Keep in mind that the electron density is large nea nucleus for hydrogen atom, indicating that the electron is most likely to be foun this region. The electron density decreases rapidly as the distance from the nuc increases.

An atomic orbital, therefore, has a characteristic energy, as well a characteristic distribution of electron density (characteristic shape). The Schrodinger equation works nicely for the simple hydrogen. The Schrodinger equation cannot be solved exactly for a multi-electron atom.

The numbers which completely describe the behavior (energy, size, shape, position and orientation or arrangement) of orbitals are called quantum numbers.

These numbers are derived from the mathematical solution of the Schrödinger equation for the hydrogen atom. They are called the principal quantum number, the azimuthal quantum number, and the magnetic quantum number. These quantum numbers are used to describe the energy level of the orbital and the three dimensional shape of the region in space occupied by a given electron. A fourth quantum number–the spin quantum number refers to a magnetic property of electrons called spin.

2.6.1 Principal Quantum Number

Number which determines the distance of electron from the nucleus (size) and its energy is called principal quantum number. It is shown by n. Its values are non-zero, positive integers up to infinity.

$n = 1, 2, 3, 4, 5, 6, 7, \ldots \infty$.

The values of 'n' can also be shown by letters K, L, M, N, O, P and Q respectively.

Table 2.4: Total Number of Orbitals and Electrons in a Shell.

Value of n	1	2	3	4	5	6	7
Letter used	K	L	M	N	O	P	Q
Total number of orbitals	1	4	9	16	25	36	49
Maximum number of electrons	2	8	18	32	50	72	98

Keep in Mind:

- Total number of orbitals in the given shell can be calculated by taking square of principal quantum number (n^2) of that shell.
- The maximum number of electrons in a shell can be calculated by $2n^2$ formula.
- Greater the value of 'n' greater will be the distance of electron from the nucleus and greater will be the size of an atom and vice versa.
- Greater the value of 'n' greater will be the energy of electron and vice versa.
- In the case of the hydrogen atom or single-electron atomic ions, such as He^{1+} and Li^{2+}, n is the only quantum number determining the energy. For other atoms, the energy also depends to a slight extent on the azimuthal quantum number.

2.6.2 Azimuthal Quantum Number

Numbers which determine the shape of an orbital and the energy of an electron, b[ut] to lesser extent than 'n' is called azimuthal quantum number. It is shown by l. It[s] values are always positive and in small whole numbers. Its values range from 0, 1, 2 and 3 ------- up to n – 1. If

n = 1 then l = (1 – 1) = 0	It shows	1s	Subshell
n = 2 then l = (2 – 1) = 0,1	It shows	2s, 2p	Subshells
n = 3 then l = (3 – 1) = 0,1,2	It shows	3s, 3p, 3d	Subshells
n = 4 then l = (4 – 1) = 0,1,2,3	It shows	4s, 4p, 4d, 4f	Subshells

The co-efficient of subshells 1,2,3,4 show the number of shells to which th[e] subshells belong.

Table 2.5: Total Number of Orbitals and Electrons in a subshell

Value of l	0	1	2	3	4	5
Letter used	s	p	d	f	g	h
Total number of orbitals	1	3	5	7	9	11
Total number of electrons	2	6	10	14	18	22

Total number of orbitals in a subshell can be determined by the formula, $2l+1$ and the total number of electrons in a subshell can be calculated by the form[ula] $2(2l+1)$.

Each shell consists of one or more subshells or sub-levels. The number [of] subshells in a shell is equal to the value of n. For example in the first shell (n = 1) there is only one subshell which corresponds to $l = 0$. There are two subshells (l = 0, 1) in the second shell (n = 2), three (l = 0, 1, 2) in third shell (n = 3) and so on. Ea[ch] subshell is assigned an azimuthal quantum number (l).

Different subshells are usually represented by letter rather than by numb[ers] following the order s, p, d, f and g. (Historically, the letters s, p, d, and f origina[ted] from the use of the words sharp, principal, diffuse and fundamental which ha[d] definite meanings in spectroscopy.) After f, successive subshells are design[ated] alphabetically: g, h and so on. The values of azimuthal quantum number also tel[l] about shape of orbitals (s-orbital has spherical shape, p has dumbbell shape, d h[as] sausage and f has complicated shape).

2.6.3 Magnetic Quantum Number

Number which explains the orientation (arrangement) of the orbital in spac[e] called magnetic or orientation quantum number. It also shows magnetic prope[rty] of electrons. It is shown by m. Its values are changing from positive to negative through zero. Within a subshell, the value of m depends on the value of the angular momentum quantum number, l. For a certain value of l, there are (2l + 1) integral values of m, as follows:

$+l, (+l-1), \ldots 0 \ldots (-l+1), -l$ or

$m = 0, \pm 1, \pm 2, \ldots$ or

$m = +2, +1, 0, -1, -2$

For s subshell, $l = 0$, then $m = 0$

There is only one orbital in the s-subshell. This orbital has same orientation along x, y and z-axis.

For p subshell, $l = 1$, then $m = [(2\times1)+1]$ or three values of m, namely, +1, 0, −1.

It means there are three different orbitals (px, py and pz) in the p subshell. The orbitals have the same shape but different orientations in space. In addition, all orbitals of a given subshell have the same energy.

For d subshell, $l = 2$, then $m = [(2\times2)+1]$ or five values of m, namely, +2, +1, 0, −1, −2. It means there are five different orbitals (dxy, dyz, dxz, dx^2-y^2 and dz^2) in the d subshell. All of these orbitals have same energy.

2.6.4 Spin quantum number

An electron spins around its own axis, much in a similar way as earth spins around its own axis while revolving around the sun. Number which shows the direction of spin of an electron around its own axis is called spin quantum number. It is also called spin magnetic quantum number. It is denoted by m_s where, the subscript *s* stands for spin. It has two values +1/2 and −1/2. The spins are also designated as ↑ or ↓. The upward arrow and the value +1/2 show that the electron spins in anticlockwise direction. The downward arrow and the value −1/2 show that the electron spins in clockwise direction.

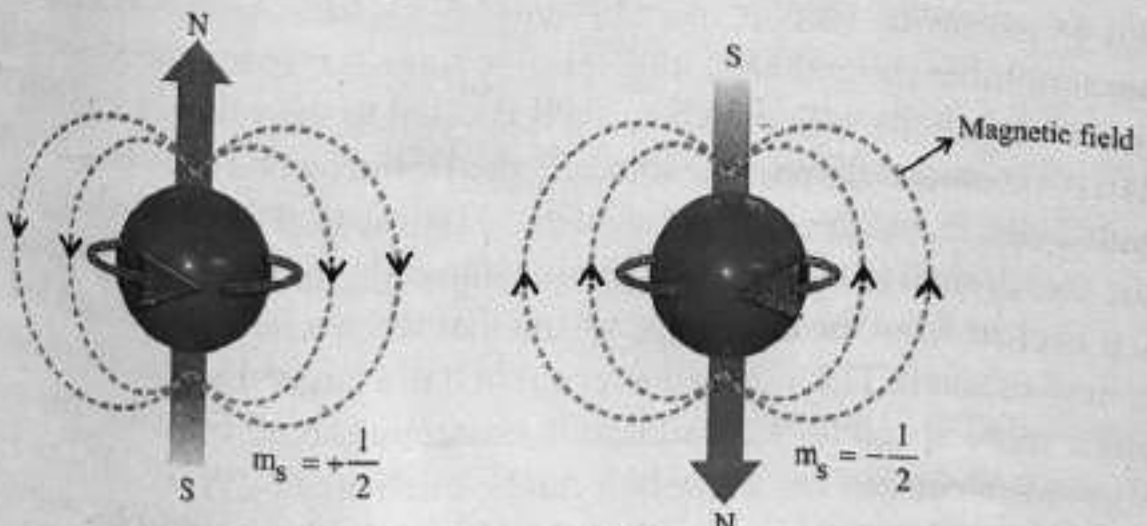

Figure 2.17: Spinning of electrons

Table 2.6: Relationship Between Shells, Subshells and Orbitals

Principal Quantum Number (n)	Azimuthal Quantum Number (l)	Subshell Designation	Magnetic Quantum Number (m)	Number of Orbitals in the subshell	Total Number of Orbitals in the Shell	Total Number of Electrons in a Shell
1	0	1s	0	1	1	2
2	0	2s	0	1		
	1	2p	1,0, −1	3	4	8
3	0	3s	0	1		
	1	3p	1,0, −1	3		
	2	3d	2,1,0, −1, −2	5	9	18
4	0	4s	0	1		
	1	4p	1,0, −1	3		
	2	4d	2,1,0,−1,−2	5		
	3	4f	3,2,1,0,−1,−2,−3	7	16	32

Shells, Subshells and Orbitals

A group of subshells with the same value of principal quantum number (n) is know as a shell. It is also recognized as orbit or energy level. The shells are designated the letters K, L, M, N, O, P, and Q, counting from the nucleus outwards. The principal quantum numbers (n) are1,2,3,4,5,6,7, ... respectively. The larger t value of 'n' the higher is the energy of the shell and vice versa. The number electrons in a shell is calculated by $2n^2$ formula. First shell (n = 1) has 2, second sh (n = 2) has 8 and third shell (n = 3) has 18 electrons.

Each principal energy level (shell) is divided into sub-levels. They are a known as subshells. One or more orbitals which have same values of princi quantum number (n) and azimuthal quantum number (l) are called subshells. T number of subshells within a given shell is equal to the value of n. Thus, the fi shell (n = 1) consists of only one subshell, the 1s; the second shell (n = 2) consis two subshells, 2s and 2p; the third shell (n = 3) consists of three subshells, 3s, 3p 3d; the fourth shell (n = 4) consists of four subshells, 4s, 4p, 4d and 4f, and so f Now it is clear from the above discussion that when a new shell is added, we add a new subshell. This is because; each shell to a larger distance from the nu provides more space for new subshells containing more orbitals. The maxi number of electrons in a subshell can be calculated by $2(2l+1)$. The s-sub has room for 2 electrons, the p-subshell has room for 6 electrons, the d-sub has room for 10 electrons, and the f-subshell has room for 14 electrons and so on. These may be shown as s^2, p^6, d^{10}, and f^{14}. A convenient way to designate such a configuration is to write the shell and subshell designation and add a superscript to denote the number of electrons occupying that subshell. For example, the electronic configuration of the calcium atom is written as follows:

$${}_{20}Ca = 1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2$$

Each subshell has specific number of orbitals. The number of orbitals per subshell depends on the type of subshell, but not on the value of n. The number of orbitals in a subshell is calculated by the formula $2l + 1$. Thus each s-subshell ($l = 0$) contains one orbital; each p-subshell ($l = 1$) contains three orbital; each d-subshell (l=2) contains five orbital, and so on. The orbitals of the same subshell in a shell have same energies and are called degenerate orbitals.

If two electrons in an atom have the same principal quantum number, the same angular momentum quantum number, and the same magnetic quantum number, the electrons are said to be in the same orbital.

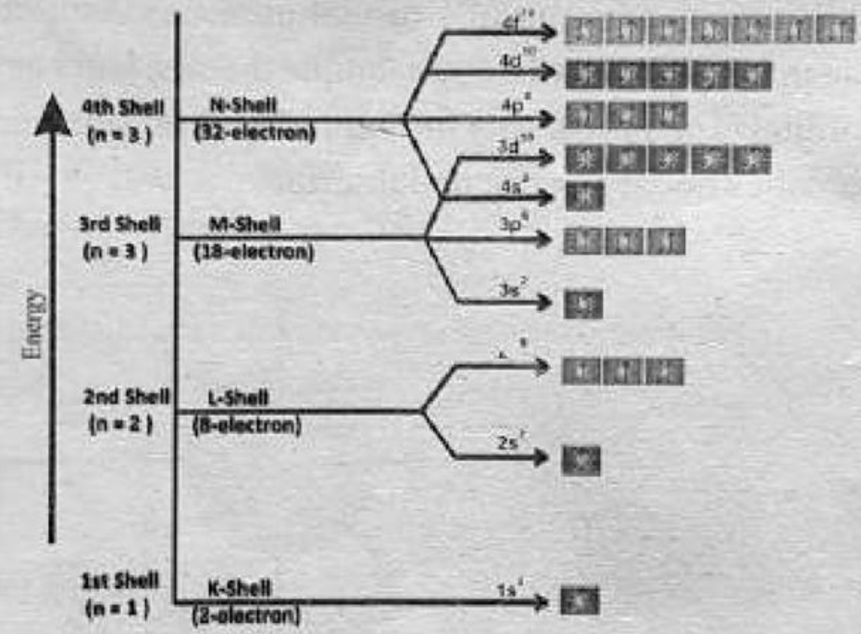

Figure 2.18: The arrangement of shells, subshells and orbitals in an atom

2.6.5 Shapes of s, p, and d-Orbitals

The shapes of orbitals have no physical existence. These are the regions in space where probability of finding an electron is very high. But these regions have no definite boundaries. Let us look the shapes of the most important orbitals that are actually occupied in known elements. Their shapes help us visualize how the electron density is distributed around the nucleus.

Shape of s-orbitals

Recall that the azimuthal quantum number for s-subshells is 0; hence, it must have magnetic quantum number 0. Thus there is only one *s* orbital in each shell. All s-orbitals have spherical shapes and are shown by circles. The probability of finding an s electron at a given distance from the nucleus does not depend on direction. It depends only on the distance from the nucleus. The electron density is high near the nucleus for an s orbital. It decreases sharply as distance from the nucleus increases, it never goes to zero, even at a large distance. If you ask someone where the electron is, he or she could not show the exact position of electron. This means that an atom does not have a definite boundary and definite shape. However, we usually draw a line around the outer edge enclosing the volume where an electron spends most (say, 95%) of its time. The space where the probability of finding the electron is maximum is called an orbital. The 1s orbital represented in this manner is merely a sphere. All s orbitals (2s, 3s, 4s, and so forth) are spherical in shape but differ in size. The size and energy of s-orbital increases with increase in the value of principal quantum number (n). For example the size and energy of 2s orbital is larger than 1s orbital. The probability of finding electron between two orbitals is zero. This plane is called nodal plane or nodal surface.

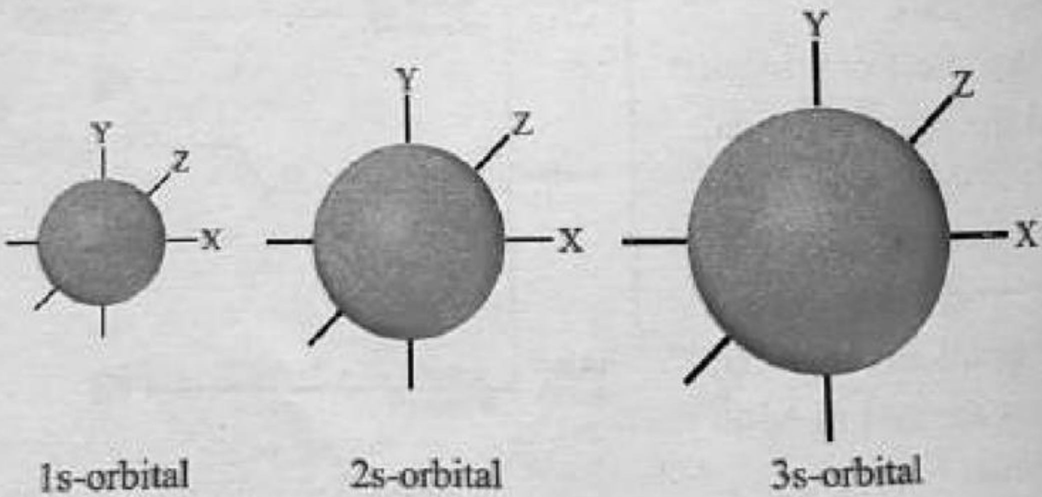

Figure 2.19: Representation of the three s-orbials of the lowest energy

Shapes of p-orbitals

As we know that the p-orbitals start with the principal quantum number n=2. Beginning with the n=2 shell, the value of azimuthal quantum number for p subshell is 1; therefore, the possible values of magnetic quantum number for p subshell are +1, 0 and −1. The three values of magnetic quantum number show that the p-orbitals have three orientations in space i.e. along x, y and z-axis. We therefore have three 2p orbitals: $2p_x$, $2p_y$ and $2p_z$, which are oriented in space at 90° angle to one another along the three coordinate axes x, y, and z. These three p-orbitals are identical in size, shape, and energy; they differ from one another only in orientation

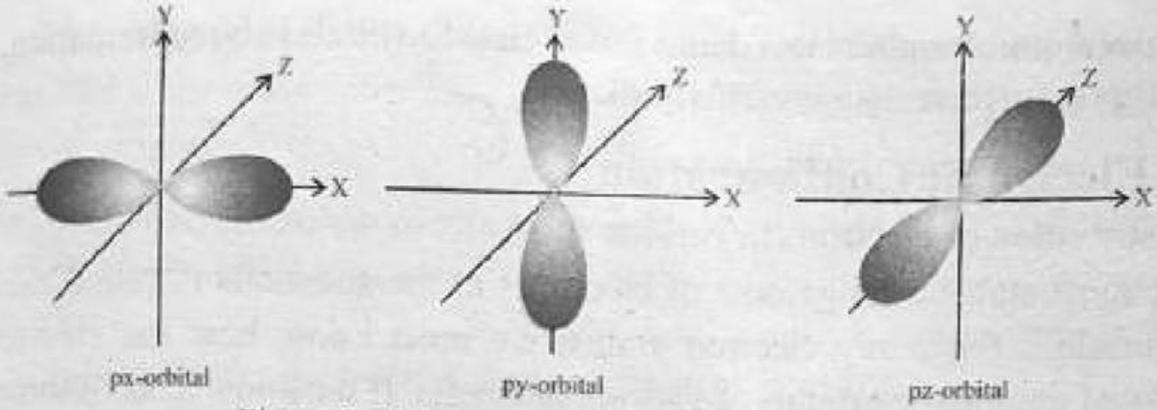

Figure 2.20: Representation of three p-orbitals

Shapes of d-orbitals

As you know that the d orbitals start with the principal quantum number $n=3$. When $n=3$ and, $l=2$, then $m=+2, +1, 0, -1, -2$. As there are five values of m for d-subshell. The d-orbitals are, therefore, of five types (d_{xy}, d_{yz}, d_{xz}, $d_{x^2-y^2}$ and d_{z^2}). Each d-orbital has clover leaf shape except d_{z^2} which has dumb-bell shape. The orbital d_{z^2} has two egg shaped lobes and an extra doughnut shape (ring shape) in the center, while other four orbitals have four egg shaped lobes. The probability of electron density is zero on the plane where the lobes touch each other. The d-orbitals of the same shell (3d orbitals) in an atom have same energy. The d-orbitals of 4^{th} and higher shells have shapes similar to 3d orbital, but differ in energy and size. They are shown as:

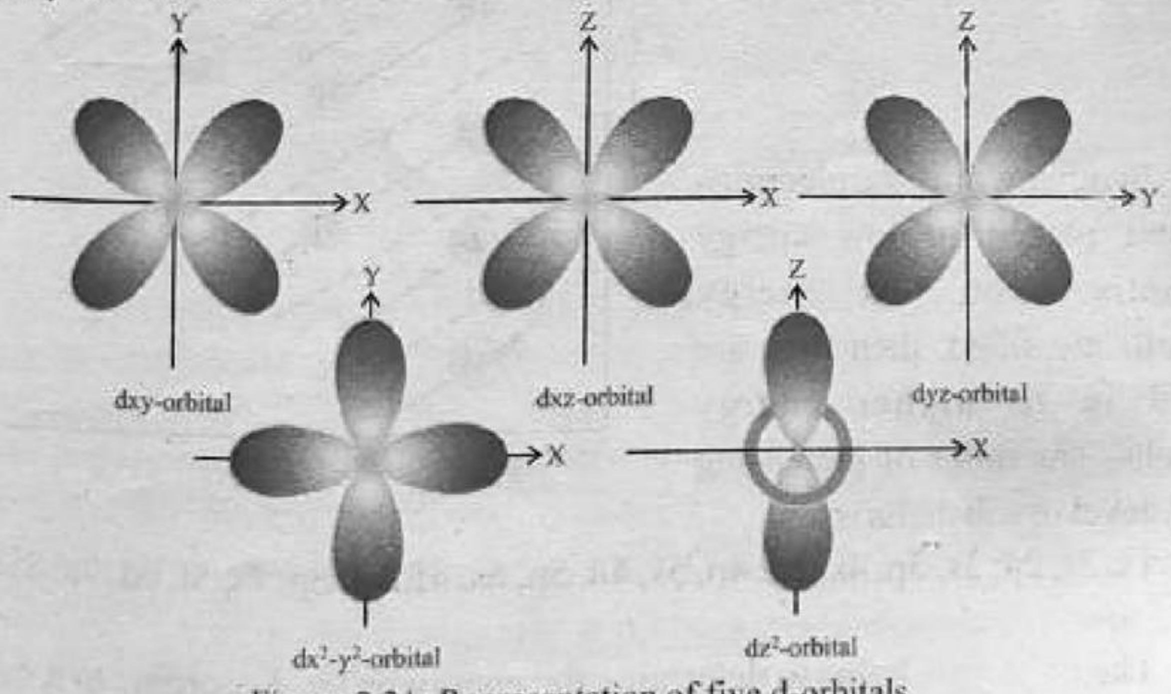

Figure 2.21: Representation of five d-orbitals

The fourth shell (n = 4) contains four subshells specified by s, p, d and f. There are seven equivalent f-orbitals. Each orbital has eight lobes. The shapes of the orbitals are even more complicated than those of the d-orbitals. Most of the elements (atomic numbers less than 57) don't use f-orbitals in bond formation, so we do not represent their shapes in this book.

2.7 Electronic Configuration

The distribution of electrons in various subshells in the increasing energy level to get the most stable arrangement of electrons in the subshells is called electronic configuration. For many electron atoms, we must know how the electrons are distributed among the orbitals of various subshells. If we know a set of three rules then we will be able to predict for each element which orbitals are occupied by electrons. The rules for distribution of electrons are as follows:

2.7.1 Aufbau Principle

The aufbau principle helps us to assign the electronic configuration to the atoms of different elements. Aufbau is a German word that means "building up". Because of this it is also known as Building up Principle. This principle states that, "The electrons are added to subshells in the order of increasing energy level".

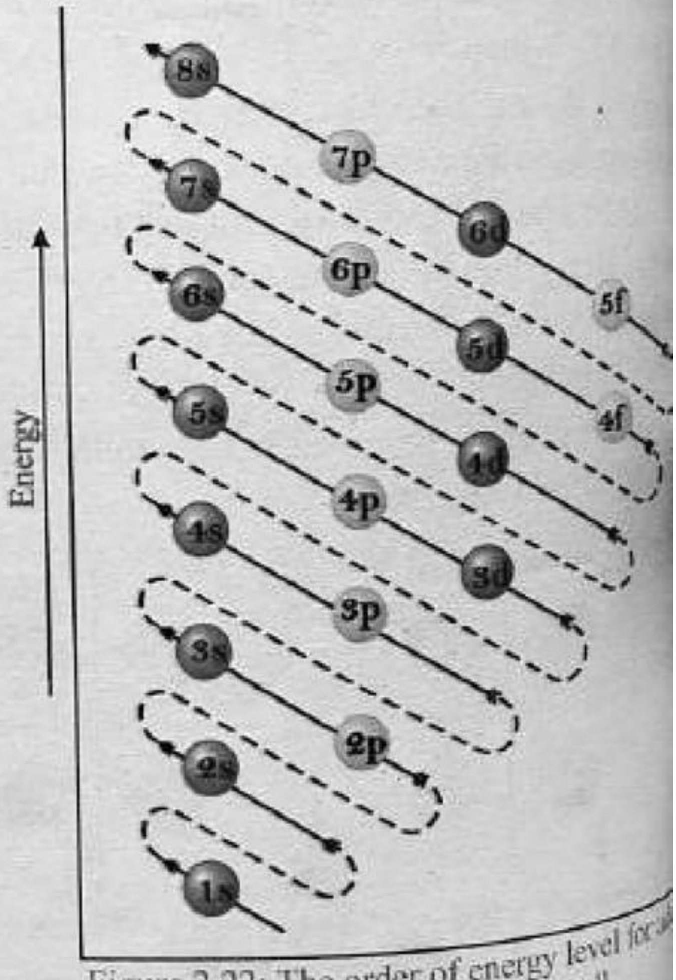

Figure 2.22: The order of energy level for filling of electrons into subshell

In other words the electrons are first placed in low energy subshells when low energy subshells are filled, then they are placed in to higher energy subshells. The order of increasing energy level of subshells is:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, 8s and so on.

The n + *l* rule helps to determine the energy order. According to n + *l* rule the electron will first enter into that subshell which has lower value of n + *l*. If n + *l* values for two or more subshells are same, then electron will enter into that subshell which has lower value of *n*.

Table 2.7: n + l values for some subshells

Subshell	n + l value	Subshell	n + l value
1s	1 + 0 = 1	3d	3 + 2 = 5
2s	2 + 0 = 2	4s	4 + 0 = 4
2p	2 + 1 = 3	4p	4 + 1 = 5
3s	3 + 0 = 3	4d	4 + 2 = 6
3p	3 + 1 = 4	4f	4 + 3 = 7

2.7.2 Pauli Exclusion Principle

Wolfgang Pauli
(1900-1958)

In 1926, an Austrian scientist Wolfgang Pauli gave the exclusion principle. According to this principle, no two electrons in the same orbital of an atom can have the same values of four quantum numbers. It means an orbital can hold at the most two electrons which have the same value of three quantum numbers n, l and m, but must have the different values of spin quantum number i.e. opposite spins (↑↓). For example, Helium atom has two electrons in 1s orbital. The spin of these electrons should be in opposite direction (↑↓). The parallel spin (↑↑ or ↓↓) of electrons is not possible. The values of four quantum numbers for both electrons of helium are given in the table.

Table 2.8: Values of four Quantum Numbers for two Electrons of same orbital

Principle Quantum Number (n)	Azimuthal Quantum Number (l)	Magnetic Quantum Number (m)	Spin Quantum Number(m_s)	
1	0	0	+1/2	For first electron
1	0	0	−1/2	For second electron

2.7.3 Hund's Rule

Friedrich Hund
(1896-1997)

In 1927, the German physicist Friedrich Hund found a rule for the determination of the lowest energy arrangement of electrons in a subshell. Hund's rule states that, "When two or more degenerate orbitals (same energy orbitals) are available, then the electrons should be placed in separate orbitals with same spin rather than to put them in same orbital with opposite spin".

As we know p-subshell has three, d-subshell has five and f-subshell has seven orbitals. The pairing of electrons begins in the p-orbitals only when the fourth electron enters into p-orbitals. In case of d and f-orbitals the pairing of electrons begins with the entry of sixth and eighth electron respectively. Hund's rule results from the fact that electrons repel one another and therefore remain as far apart as possible. They can be lower in energy if they are in different orbitals. The electronic configuration in the orbitals of same element is given in table 2.9.

Applications of Rules

i) These rules are used to write electronic configuration of elements.

ii) These rules are used to predict valency.

iii) These rules show number and type of half-filled orbitals.

iv) These rules show orbitals involved in bond formation.

2.7.4 Writing the Electronic Configuration of Elements

Before we assign the electronic configurations to atoms of the different elements, we have to know the methods of representing these configurations. There are two different ways (methods) for writing the electronic configuration of an atom.

i) In this method, we write the symbol for the occupied subshell and add a superscript to indicate the number of electrons in that subshell and then we write the principal quantum number before the particular subshells. The electronic configuration of Helium atom is shown in figure 2.23. The electronic configuration of nitrogen atom can be written as $1s^2\ 2s^2 2p^3$.

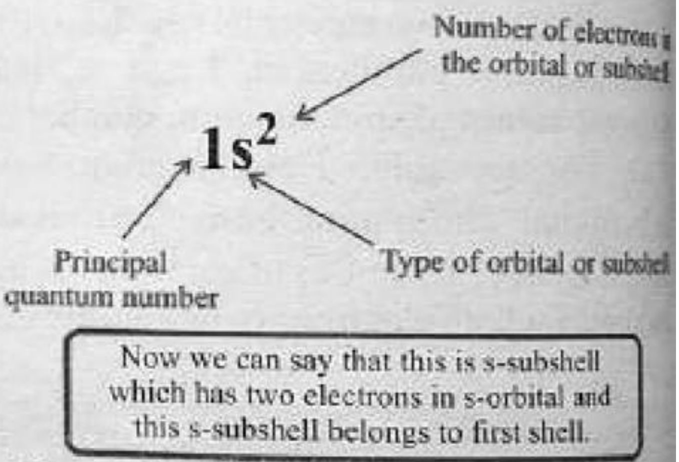

Figure 2.23: Method of writing the electronic configuration

ii) In this method, each orbital of the sub-shell is represented by a box and the electron is shown by an arrow (↑). The arrow points up when electron spins anticlockwise and down when electron spins clockwise. If an orbital contains only one electron, an arrow pointing upward (↑) is placed in the box. If an orbital contains two electrons, the second arrow pointing downward (↓) is placed in the box. The two electrons in orbital which have opposite spins are said to be paired. The single electron in an orbital which has no partner of opposite spin is said to be unpaired electron. The priority is given to this method over the first because it represents all the four quantum numbers.

Table 2.9: Electronic Configurations and Orbital Diagrams for First 18 Elements

Element	Atomic Number	Electronic Configuration	Orbital 1s	2s	2p	3s	3p
H	1	$1s^1$	[↑]				
He	2	$1s^2$	[↑↓]				
Li	3	$1s^2\,2s^1$	[↑↓]	[↑]			
Be	4	$1s^2\,2s^2$	[↑↓]	[↑↓]			
B	5	$1s^2\,2s^2\,2p^1$	[↑↓]	[↑↓]	[↑][ ][ ]		
C	6	$1s^2\,2s^2\,2p^2$	[↑↓]	[↑↓]	[↑][↑][ ]		
N	7	$1s^2\,2s^2\,2p^3$	[↑↓]	[↑↓]	[↑][↑][↑]		
O	8	$1s^2\,2s^2\,2p^4$	[↑↓]	[↑↓]	[↑↓][↑][↑]		
F	9	$1s^2\,2s^2\,2p^5$	[↑↓]	[↑↓]	[↑↓][↑↓][↑]		
Ne	10	$1s^2\,2s^2\,2p^6$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]		
Na	11	$1s^2\,2s^2\,2p^6\,3s^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑]	
Mg	12	$1s^2\,2s^2\,2p^6\,3s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	
Al	13	$1s^2\,2s^2\,2p^6\,3s^2\,3p^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][ ][ ]
Si	14	$1s^2\,2s^2\,2p^6\,3s^2\,3p^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][ ]
P	15	$1s^2\,2s^2\,2p^6\,3s^2\,3p^3$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][↑]
S	16	$1s^2\,2s^2\,2p^6\,3s^2\,3p^4$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑][↑]
Cl	17	$1s^2\,2s^2\,2p^6\,3s^2\,3p^5$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑]
Ar	18	$1s^2\,2s^2\,2p^6\,3s^2\,3p^6$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]

Instead of writing out the whole electronic configuration of an element, we write the condensed electronic configuration by writing the electronic configuration of the previous noble gas. The electronic configuration of the noble gas is represented by its chemical symbol in brackets. For example, the electronic configuration of silicon is written as [Ne]$3s^23p^2$.

Where, [Ne] denotes the "neon core." Similarly we can write the electronic configuration of calcium as [Ar]$4s^2$.

Table 2.10: The Condensed form of Electronic Configurations from Potassium (Z = 19) to Krypton (Z = 36)

Element	Symbol	Atomic Number	Electronic Configuration
Potassium	K	19	[Ar]$4s^1$
Calcium	Ca	20	[Ar]$4s^2$
Scandium	Sc	21	[Ar]$4s^23d^1$
Titanium	Ti	22	[Ar]$4s^23d^2$
Vanadium	V	23	[Ar]$4s^23d^3$
Chromium	Cr	24	[Ar]$4s^13d^5$
Manganese	Mn	25	[Ar]$4s^23d^5$
Iron	Fe	26	[Ar]$4s^23d^6$
Cobalt	Co	27	[Ar]$4s^23d^7$
Nickel	Ni	28	[Ar]$4s^23d^8$
Copper	Cu	29	[Ar]$4s^13d^{10}$
Zinc	Zn	30	[Ar]$4s^23d^{10}$
Gallium	Ga	31	[Ar]$4s^23d^{10}4p^1$
Germanium	Ge	32	[Ar]$4s^23d^{10}4p^2$
Arsenic	As	33	[Ar]$4s^23d^{10}4p^3$
Selenium	Se	34	[Ar]$4s^23d^{10}4p^4$
Bromine	Br	35	[Ar]$4s^23d^{10}4p^5$
Krypton	Kr	36	[Ar]$4s^23d^{10}4p^6$

The electron configuration of chromium (Z = 24) is [Ar] $4s^13d^5$ instead of [Ar] $4s^23d^4$, as we might expect. Similarly the electronic configuration of copper (Z = 29) is [Ar] $4s^13d^{10}$ rather than [Ar] $4s^23d^9$. This is because the half-filled ($3d^5$) and completely filled ($3d^{10}$) subshells are more stable than partially filled subshells.

Summary of Facts and Concepts

- Atoms are the basic building blocks of matter. They are the smallest units of an element which chemically react. An atom consists of a very small, dense and positively charged central nucleus and a diffused region of negative charge around nucleus. Atoms are composed of three fundamental particles the electron, the proton, and the neutron.

- The number of protons in the nucleus of an atom of an element is called atomic number (Z). Atomic number is the identity of an atom of an element. All atoms of a given element have the same atomic number, which differs from the atomic numbers of other elements. The number of electrons is always equal to the number of protons in an atom.
- The mass number (A) is the sum of the number of protons and the number of neutrons in the nucleus of an atom. Isotopes are atoms of the same element that have the same number of protons but different mass numbers because they have different numbers of neutrons. An isotope is identified by the symbol of the element, with the mass number as a superscript to the left. Isotopes have chemical behavior identical to that of any other isotope of the same element.
- Max Planck, in 1900, gave quantum theory of radiations.
- Neil Bohr, in 1913, successfully explained spectrum of hydrogen and hydrogen like atoms. He proposed that the electron revolves around the nucleus in the circular path with a definite amount of energy. He called these paths orbits or shells.
- Spectrum is the bands of different colours which are produced by passing light through prism. Rainbow is the best example of spectrum.
- X-rays are produced when fast moving electrons collide with heavy metals anode in the discharge tube. These rays were discovered by a German scientist W.C. Roentgen in 1895.
- After the failure of Bohr's atomic model, Erwin Schrodinger, in 1926, proposed an equation called Schrödinger equation to describe the electron distributions in space and the allowed energy levels in atoms.
- In a hydrogen atom and hydrogen like atoms, which contains only one electron, the energy of an orbital depends only on n. In a multi-electron atom, the energy of an orbital depends on both n and l. The lower the value of $(n+l)$ for an orbital, the lower is its energy. If two orbitals have the same $(n+l)$ values, the orbital with lower value of n has the lower energy. In addition; the spin quantum number determines the electron spin as either clock wise or anti-clock wise.
- According to Aufbau principle, the electrons are added to energy subshells in the order of increasing energy level.
- Pauli Exclusion Principle states that no two electrons in the same orbital of an atom can have the same values of four quantum numbers.
- Hund's rule states that the pairing of electrons in the degenerate orbitals (same energy orbitals) does not take place until each degenerate orbital has got one electron each.

Questions and Problems

Q.1. Four answers are given for each question. Select the correct one.

i) The fundamental particles of an atom are:

(a) Electron, positron, neutron (b) Electron, proton, neutron

(c) Electron, neutrino, proton (d) Electron, positron, meson

ii) Proton was discovered by:

(a) Gold Stein (b) Chadwick

(c) Thomson (d) W. Crooks

iii) The colour of the glow inside the discharge tube depends upon:

(a) Nature of discharge tube (b) Nature of the gas

(c) Nature of cathode (d) Nature of anode

iv) The mass of electron is almost equal to:

(a) Hydrogen atom (b) Proton

(c) Neutron (d) Positron

v) How many times the second orbit of hydrogen atom is away from the nucleus:

(a) Four (b) Six

(c) Nine (d) Sixteen

vi) Which one of the following elements is **NOT** radioactive:

(a) Uranium (b) Polonium

(c) Radium (d) Germanium

vii) The properties of elements are determines by:

(a) Atomic mass (b) Mass number

(c) Atomic number (d) All of these

viii) When 6s orbital is complete, the entering electron goes into:

(a) 7s (b) 6p

(c) 5d (d) 4f

ix) If n is equal to 4, then *l* is equal to:

(a) 0 (b) 0, 1

(c) 0,1,2 (d) 0,1,2,3

x) How many electrons an orbital can accommodate:

(a) 14 (b) 10

(c) 6 (d) 2

Q.2. Fill in the blanks with suitable words given in the brackets:

i) Cathode rays produce _______ on striking with heavy metals anode. (canal rays/X-rays)

ii) Mass of proton in amu is _______. (1.00727/1.00867)

iii) Pfund series of lines appear in _______ region of spectrum. (UV/IR)

iv) Mathematical value for Bohr's radius constant (a_o) is _______. (5.29 A^o/0.529 A^o)

v) Cathode rays bent toward _______ of electric field. (positive plate/negative plate)

vi) Energy is _______ when electron jumps from lower to a higher orbit. (absorbed/released)

vii) Greater the value of principle quantum number, _______ will be the size of an atom. (lesser/greater)

viii) The subshell p has _______ shape. (spherical/dumbbell)

ix) The wavelength of X-rays is _______ than microwaves. (greater/lesser)

x) Wavelength of large sized particles is very _______. (small/large).

Q.3. Label the following statements as True or False:

i) Neutrino is the fundamental particle of an atom.

ii) The electric current cannot pass through gases in the discharge tube at 760 torr.

iii) The mass of electron in kg is 9.11×10^{-31}.

iv) The charge to mass ratio of canal rays depends upon the nature of gas in the tube.

v) Planck's equation is $E = mc^2$.

vi) The electronic configuration of H^- is $1s^2$.

vii) If n = 4, then *l* is equal to 0, 1, 2.

viii) Orbit gives the idea of plane motion of electrons.

ix) Monitor of computer is anode rays tube.

x) The space where probability of finding the electron between two orbitals is zero is called nodal plane.

Q.4. What is discharge tube? Describe the experiment which led to the discovery of electron.

Q.5. Give the characteristic properties of cathode rays.

Q.6. Answer the questions given below:

i) The cathode rays are produced when pressure inside the discharge tube is reduced and high voltage is applied.

ii) The charge-to-mass ratio of cathode rays remains same, no matter which gas is used in the discharge tube.

iii) The charge-to-mass ratio of cathode rays is equal to that of electron.

iv) The evidence that cathode rays consist of negatively charged particles.

v) Electrons are the elementary particles of all the matter.

Q.7. What are canal rays? Give reason for the production of canal rays.

Q.8. What are the properties of canal rays?

Q.9. Explain the following with reasons:

i) The positive rays are also called canal rays.

ii) The canal rays depend upon the nature of gas.

iii) The e/m values of canal rays for different gases are different.

iv) The e/m value of cathode rays is 1836 times greater than positive rays that are obtained from hydrogen gas.

Q.10. How were neutrons discovered? Describe the properties of neutrons.

Q.11. Slow neutrons are more effective than fast neutrons, how?

Q.12. Explain J. J. Thomson experiment for determining the e/m ratio of electron.

Q.13. Compare the properties of fundamental particles of atom.

Q.14. Which two types of subatomic particles must be present in equal number for an atom to be neutral?

Q.15. What is the atomic number of an atom that has 17 protons, 17 electrons and 18 neutrons? Also calculate its mass number.

Q.16. An atom with mass number of 36 contains four more neutrons than protons. What is the atomic number and name of this atom?

Q.17. Discuss Rutherford's experiment for the discovery of nucleus.

Q.18. Write main points of Rutherford's atomic model. What are the defects of this model.

Q.19. What are the most important points of Planck's quantum theory? Explain what a quantum is?

Q.20. What is the relationship between?

a) Frequency and wavelength

b) Wavelength and wavenumber

Q.21. Define the terms given below:

(a) Frequency

(b) Wavelength

(c) Wavenumber

(d) Atomic number

(e) Amplitude

Q.22. What are the postulates of Bohr's atomic model? What are the merits and demerits of this concept?

Q.23. Derive an expression for the radius of nth orbit of hydrogen atom with the help of Bohr's model.

Q.24. Derive an expression for calculating the energy of an electron in the n^{th} orbit of hydrogen atom with the help of Bohr's model.

Q.25. Derive the formulas for calculating the energy difference (ΔE), frequency of photon and wavenumber of photon.

Q.26. Answer the following questions:

a) The distance between different orbits goes on increasing when we move from lower to higher orbits.

b) Energy of electron is inversely proportional to the square of number of orbits (n^2).

c) The energy of higher orbits is greater than lower orbits.

d) The energy of electron at an infinite distance from the nucleus is zero.

e) The radius of cation is smaller than its parent atomic radius.

f) Velocities of electrons in higher orbits are less than those in the lower orbits of hydrogen atom.

g) Why the size of helium ion (He^+) is smaller than hydrogen atom as both have same number of electrons in the first shell?

Q.27. What do you know about Zeeman Effect and Stark Effect?

Q.28. What is spectrum? Explain the spectrum of hydrogen atom.

Q.29. What are X-rays? How are they produced? Describe the properties and uses of X-rays.

Q.30. Explain the role of Mosley's law in determining the atomic numbers of different elements.

Q.31. Define energy level. What is the difference between ground state excited state?

Q.32. How can you define orbit and orbital? Explain the difference between and orbital.

Q.33. What are quantum numbers? State the significance of each quan number.

Q.34. What values of quantum numbers are assigned to the following orbitals

(a) 2s-orbital (b) 3p-orbital (c) 4d-orbital (d) 5f-orbital

Q.35. Describe the shapes of s, p, and d-orbitals. How are these orbitals relat azimuthal and magnetic quantum numbers?

Q.36. What do you know about shells, subshells and orbitals? Describe in det

Q.37. What is Aufbau principle? Arrange the subshells according to principle. Get the ground state electronic configuration of first 18 elem by using this principle.

Q.38. Discuss the following:

a) Pauli's Exclusion Principle.

b) Hund's Rule

Q.39. What is electronic configuration? Describe the basic rules and metho writing electronic configuration for the atoms of different elements.

Q.40. Answer the following question:

a) What are the total number of subshells and orbitals in an atom principle quantum number, $n = 4$?

b) What is the maximum number of electrons in first, second, thi fourth shells?

c) How many orbitals are in the 2p and 3p subshells?

d) Calculate the number of orbitals in $l = 4$ subshell.

e) Give the values of the quantum numbers associated with 2s, 3p orbitals.

f) What are the similarities and dissimilarities between 2p orbitals?

g) Discuss the difference between $2p_x$ and $2p_y$ orbitals.

h) Which of the following orbitals do not exist: 1s, 1p, 2p, 2d, and 4g?

i) Which subshell in each of the following pairs is higher in energy?

(i) 4p or 5s (ii) 5s or 6p (iii) 6s or 4f

j) What is the meaning of $3p^4$?

k) How many unpaired electrons are present in oxygen and silicon atoms in the ground state?

Q.41. Calculate the energy of one photon of blue light having wavelength of 490nm.

Q.42. Calculate the frequency, energy and wavenumber of a yellow light emitted from a sodium lamp which has a wavelength of 570nm.

Q.43. Explain Millikan's oil drop experiment for measurement of charge of electron.

Q.44. Calculate the ΔE when electron jumps from lower orbit (n_1) to higher orbit (n_2).

Q.45. Calculate the frequency (Hz) and wavelength (nm) of the light absorbed by hydrogen atom when an electron jumps from the $n=2$ to the $n=3$ level.

Q.46. Explain why the subshell is not full in oxygen atom and full in neon atom?

Q.47. Calculate mass of electron from e/m ratio and mass.