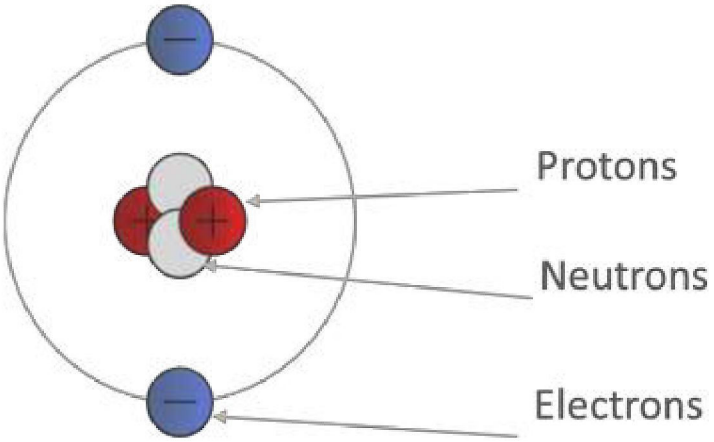
Atomic structure

- Atom consists of positively charged **NUCLEUS** at the centre and negatively charged **Electrons** revolving around it.
- Radius of an atom -- 10^{-10} m.
- Radius of the nucleus -- 10^{-15} m.
- Nucleus consists of Protons and Neutrons together called Nucleons.
- Most of the mass of an Atom is possessed by Nucleus.



John Dalton

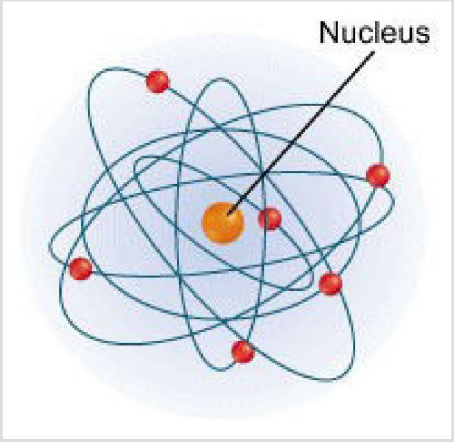
- Atoms were tiny particles that could not be divided
- Each element had its own kind of atom
- John Dalton proposed that an atom is a sphere of matter that is the same throughout.
- Marble Model

JJ Thomson

- Came up with the idea of the electron – negatively charged particle
- J.J. Thomson discovered that all atoms contain electrons, which are tiny, negatively charged particles. Thomson proposed that an atom is a sphere of positive charge. The electrons are mixed uniformly in the sphere.
- Clay with embedded spheres

Ernest Rutherford

- He hypothesized that almost all the mass and all the positive charge of an atom is concentrated in an extremely tiny nucleus at the center of the atom.



Electron

- Negatively charged sub-atomic particle
- Weight = 0.0006 atomic mass unit
- Move rapidly
- Form an electron cloud (area where electrons are likely to be)

Protons

- Positively Charged Sub-atomic particles
- Found in the nucleus
- All protons are a like
- Weight of 1 proton =

  1 atomic mass unit

Neutron

- Neutrally charged (no charge) sub-atomic particle
- Atomic weight of 1 atomic mass unit
- Found in nucleus

Calculating Neutrons

- Mass number = protons + neutrons

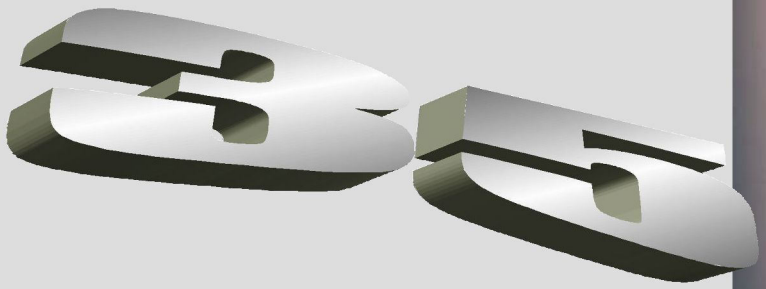
so…..

- Neutrons = mass number – protons

How many neutrons does Copper have?

Mass # = 63.546

(rounds to 64)



Neutrons = 64-29

=

Nucleus

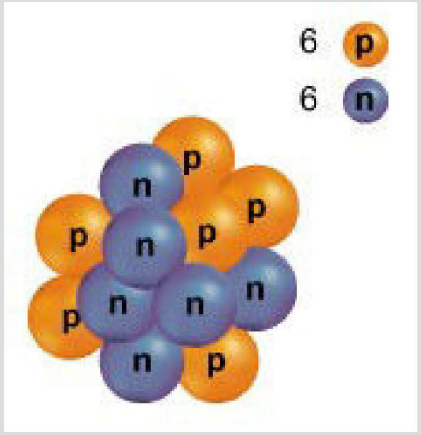
- Center or core of an atom
- Contains 99.9% of the weight of an atom
- Contains protons and neutrons
- Occupies 1 / 100,000 of the space of an atom

Atomic Number

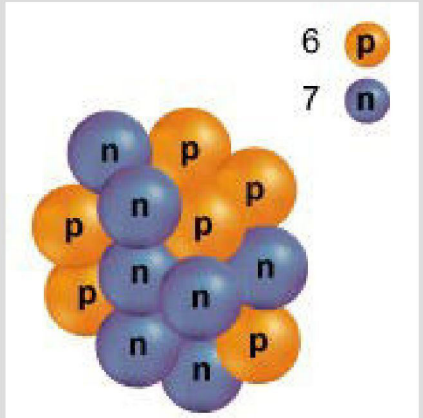
- Atomic number is the number of Protons in an atom
- All atoms of a particular element have the SAME number of protons (All Carbon atoms have 6 protons)
- In a neutral atom, the atomic number = the number of electrons

Isotopes

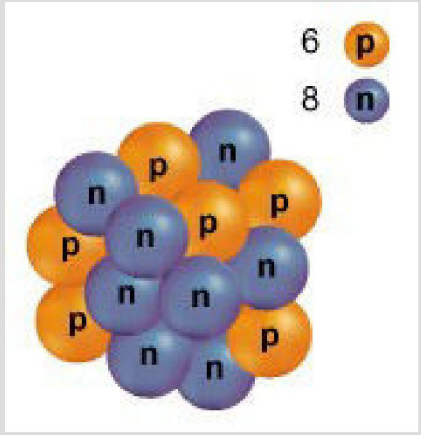
- Atoms of the same element with different numbers of neutrons.



Carbon 12

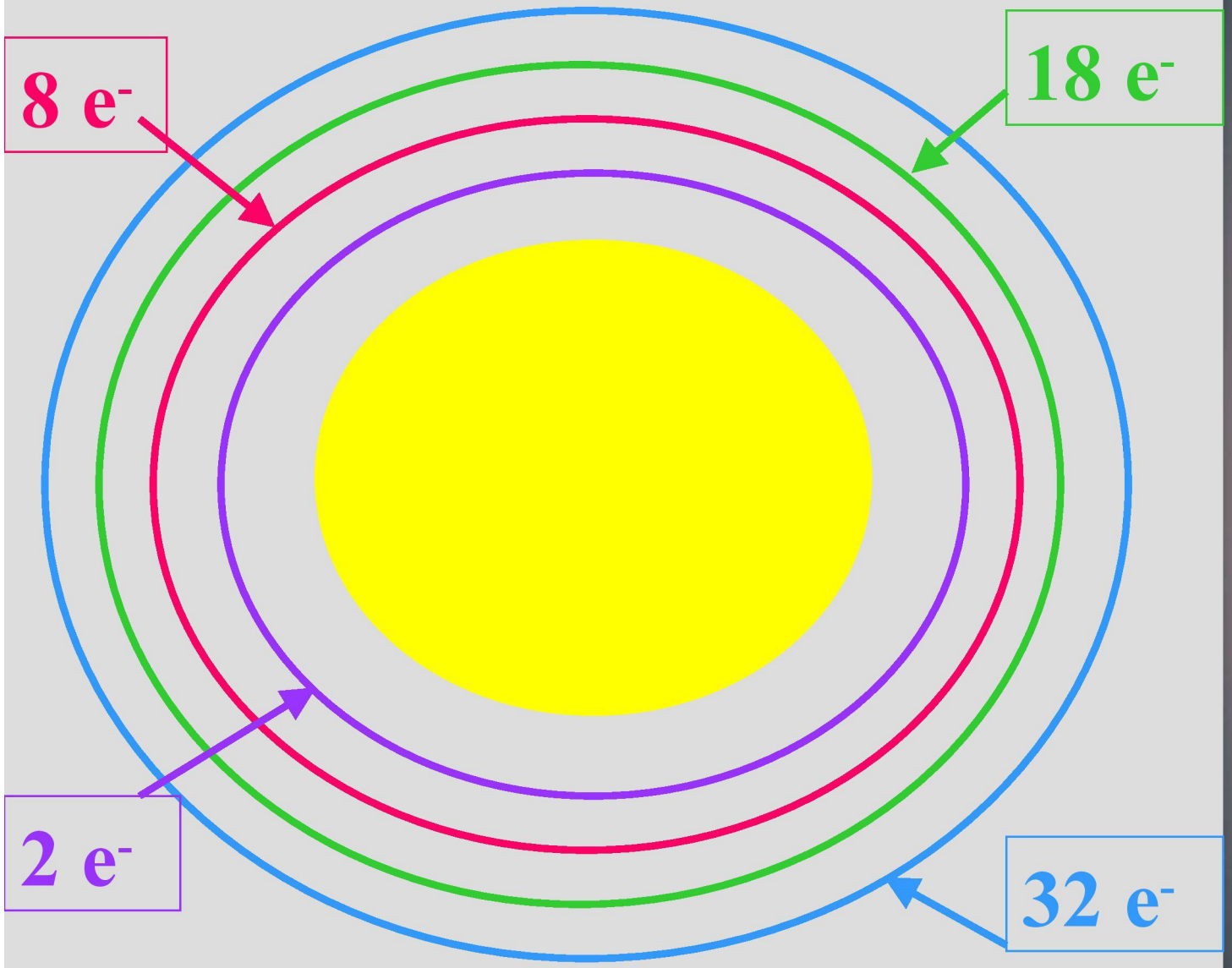


Carbon 13



Carbon 14

Electrons in Energy Levels

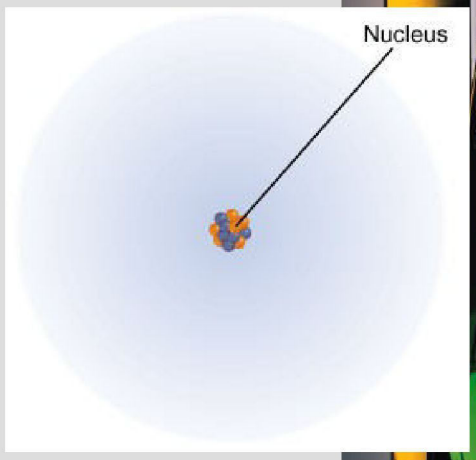


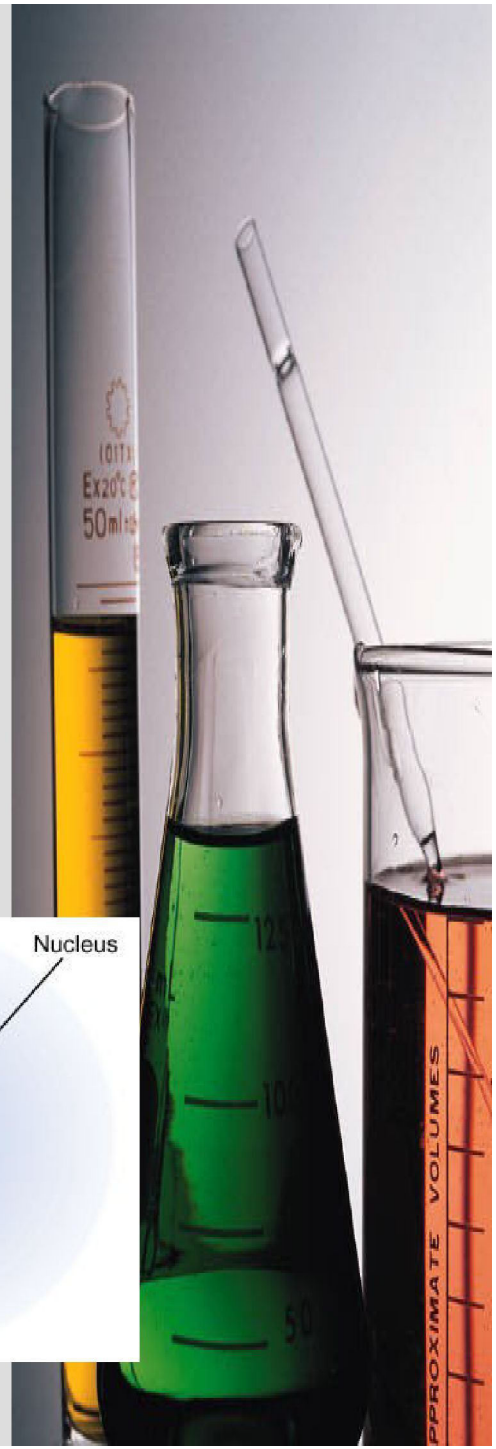
Niels Bohr

- Thought electrons traveled in fixed paths around the nucleus called energy levels.

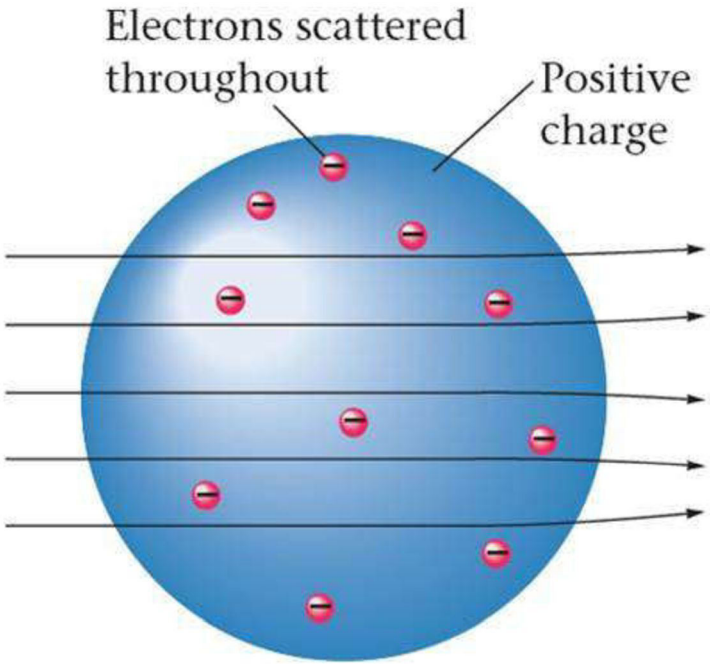
Electron Cloud

- Electrons are in random orbits around the nucleus
- Electrons move rapidly throughout the atom
- Energy Levels Still Exist

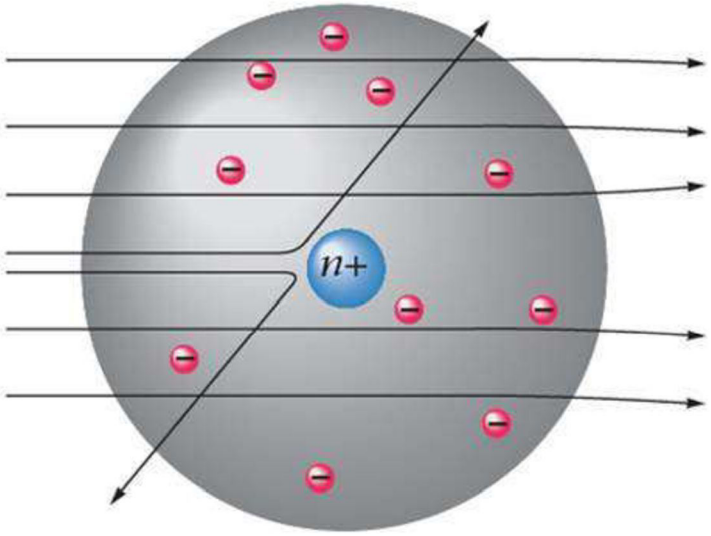




Results of the Rutherford experiment



(a) The results that the metal foil experiment would have yielded if the plum pudding model had been correct.



(b) Actual results

Theories of Atomic models:

John Dalton

- Matter is made of indivisible atoms, they are indestructible.
- All atoms of a given (same) element are identical in their physical and chemical properties.
- Atoms of different elements differ in their physical and chemical properties.
- Atoms of different elements combine in simple whole-numbers ratios to form **Molecules**
- Chemical reactions consist of the combination separation or rearrangement of atoms

- ***Limitations:*** **It could not explain**

•Why and how do atoms combine together to form compound atoms (molecules)

•The nature of forces which hold atoms together in compound atoms

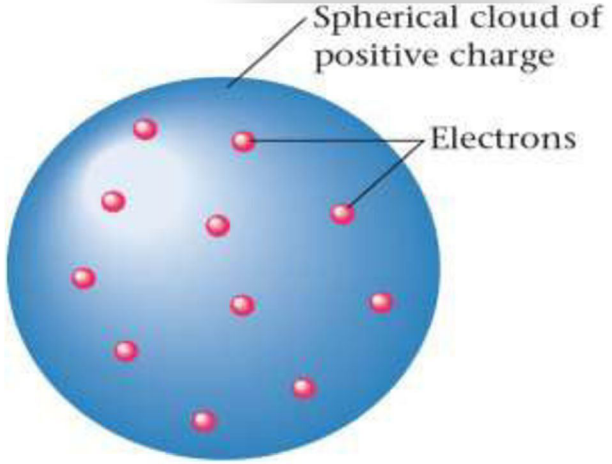
•Why atoms cannot exist in free state and why compound atoms can exist freely.

Theories of Atomic models:

J.J.THOMPSON

Plum pudding model(1904)

- Negative particles are evenly scattered throughout an atom with a positively charged mass of matter.
- Similar to that of chocolate chip icecream
- Later proved to be incorrect.



Limitations:

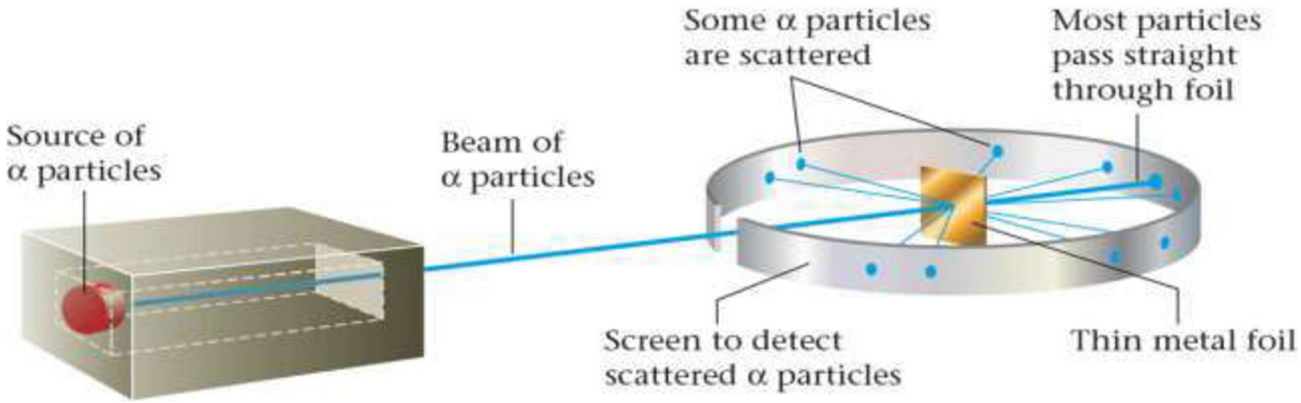
- It could not explain the result of scattering experiment explained by rhe Rutherford experiment.
- It did not have any experimental evidence in its support .

Thermionic emission, photoelectric emission and ionization were explained on this basis.

Theories of Atomic models:

RUTHERFORD

Rutherford Gold foil experiment setup:

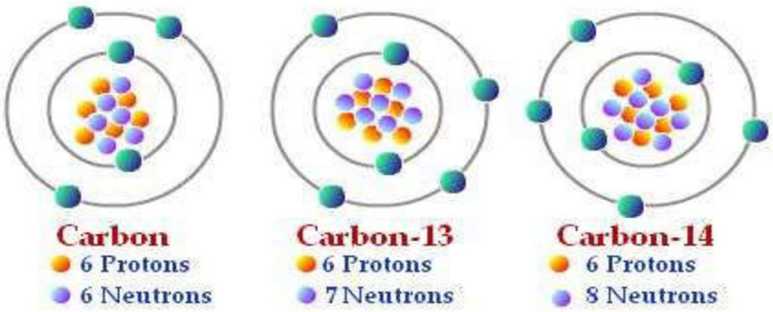


- If a thin foil metal is placed in the path of the beam, the image becomes diffuse.
- This due to the scattering of α- particles by the atoms of the foil.
- The particles scattered in various directions were counted by scintillation counter
- It was found that although most of the particles scattered through angles of the order of 1^0 or less
- But a small number say about 1 in every 10,000 scattered through 90^0 or even 180^0
- The experiment is known as Rutherford's alpha particle scattering experiment.

Classification of atoms:

* **Isotopes -** Elements having same atomic number (protons) , but different mass numbers (nucleons).

eg: ^{12}C, ^{13}C and ^{14}C



are three isotopes of the element carbon with mass numbers 12, 13 and 14 respectively. The atomic number of all carbon isotopes is 6.

* **Isobars -** Elements having same mass number , but different atomic numbers.

eg: ^{40}S , ^{40}Cl , ^{40}Ar , ^{40}K, and ^{40}Ca

are isobars containing 40 nucleons; however, they contain varying atomic number.

Conclusion of Rutherford experiment

- The whole of the positive charge of atom must be concentrated in a very small space
- Atom is mostly hollow inside
- Since α- particles are positively charged, the part of the atom deflecting them must also be positive
- Most of the mass of the atom is concentrated in the nucleus
- In this model, the mass of the atom (leaving the mass of its electrons) and its whole positive charge are concentrated at the centre of the atom in a nucleus of radius 10^{-15} m
- The electrons are distributed around the nucleus in a hollow sphere of radius 10^{-10} m

Drawback's of Rutherford's Model

Regarding stability of atom

- Electrons revolving around the nucleus have centripetal acceleration
- According to electrodynamics, accelerated charged particles radiate energy in the form of electromagnetic waves
- Hence electromagnetic waves should be continuously radiated by the revolving electrons
- Due to this continuous loss of energy of the electrons, the radii of their orbits should be continuously decreasing and ultimately the electron should fall into the nucleus
- Thus atom cannot remain stable

- **Rutherford's model also failed to explain the Line spectrum.**

Theories of Atomic models:

Niels David Bohr

- NIELS DAVID BOHR A Danish physicist who developed Bohr model of atomic structure, in which he introduced the theory of electrons orbiting around the nucleus.

Bohr's theory (Postulates)

1. Fixed circular orbits :The electrons move around the nucleus in concentric circular orbits .
2. While revolving in stable orbits, the electrons do not radiate energy in spite of their acceleration towards the centre of the orbit.
3. Each of the fixed orbits is associated with a definite amount of energy called stationary energy.

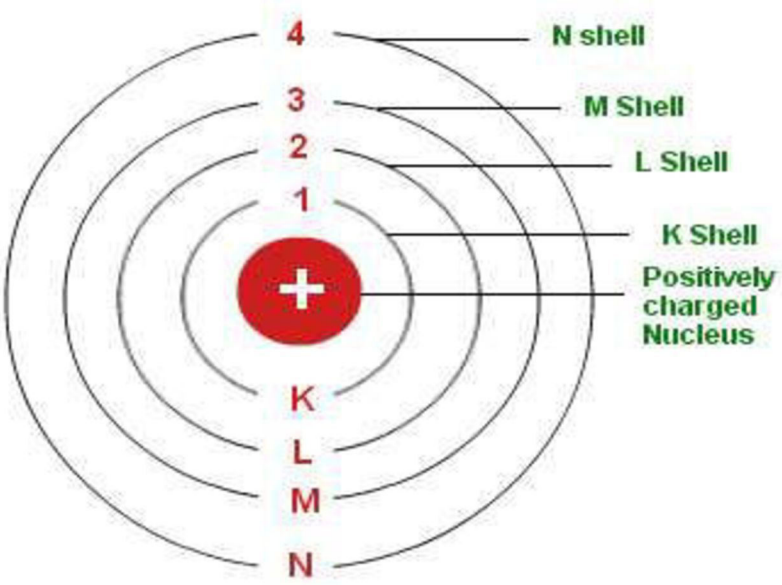
   The energy levels are numbered as 1, 2, 3, 4... or designated as K,L,M, N ...
4. Jumping of an electron from one energy level to the other (ground state and excited state) .

5. Principle of quantization of angular momentum of the moving electron an electron can move only in that orbit in which the angular momentum of the electron around the nucleus is an integral multiple of $h/2\pi$.

DISTRIBUTION OF ORBITAL ELECTRONS:

According to the model proposed by Niels Bohr in 1913

- Electrons revolve around the nucleus in specific orbits.
- They are prevented from leaving the atom by the necessary centripetal force of attraction between the positively charged nucleus and negatively charged electron.



Bohr's Atomic model

Postulates of Bohrs theory :

a) Electrons can exist in only those orbits for which angular momentum of electron is an integral multiple of **$h/2\Pi$**

(h= plancks constant 6.62×10^{-34})

b) No energy is gained or lost while an electron remains in any one of the permissible orbits.

Limitations of Bohr's Postulates

I. **No explanation for the spectra of multi electron systems:**

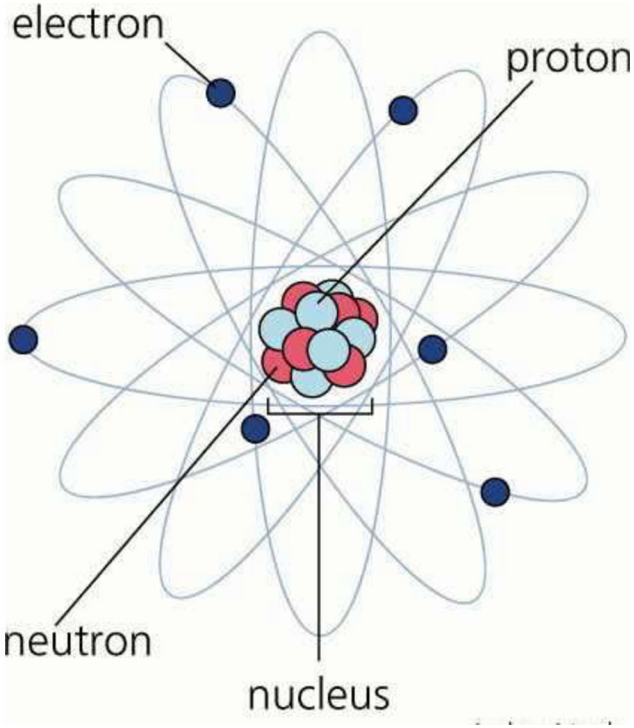
Eg: He, Li

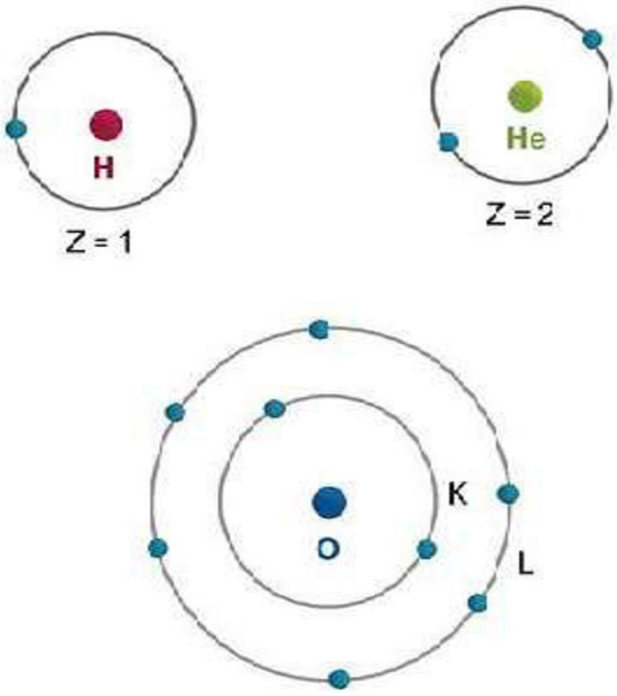
I. **No explanation of fine spectrum of atoms:**

III. **No explanation for Zeeman and Stark effect** : effect of electric and magnetic fields on the spectral atoms.

- When a magnetic field is applied on an atom, its usually observed spectral lines split. This effect is known as **Zeeman's effect**
- Spectral lines also get split in the presence of electric field. This effect is known as **Stark effect.**

Arrangement of electrons in orbitals

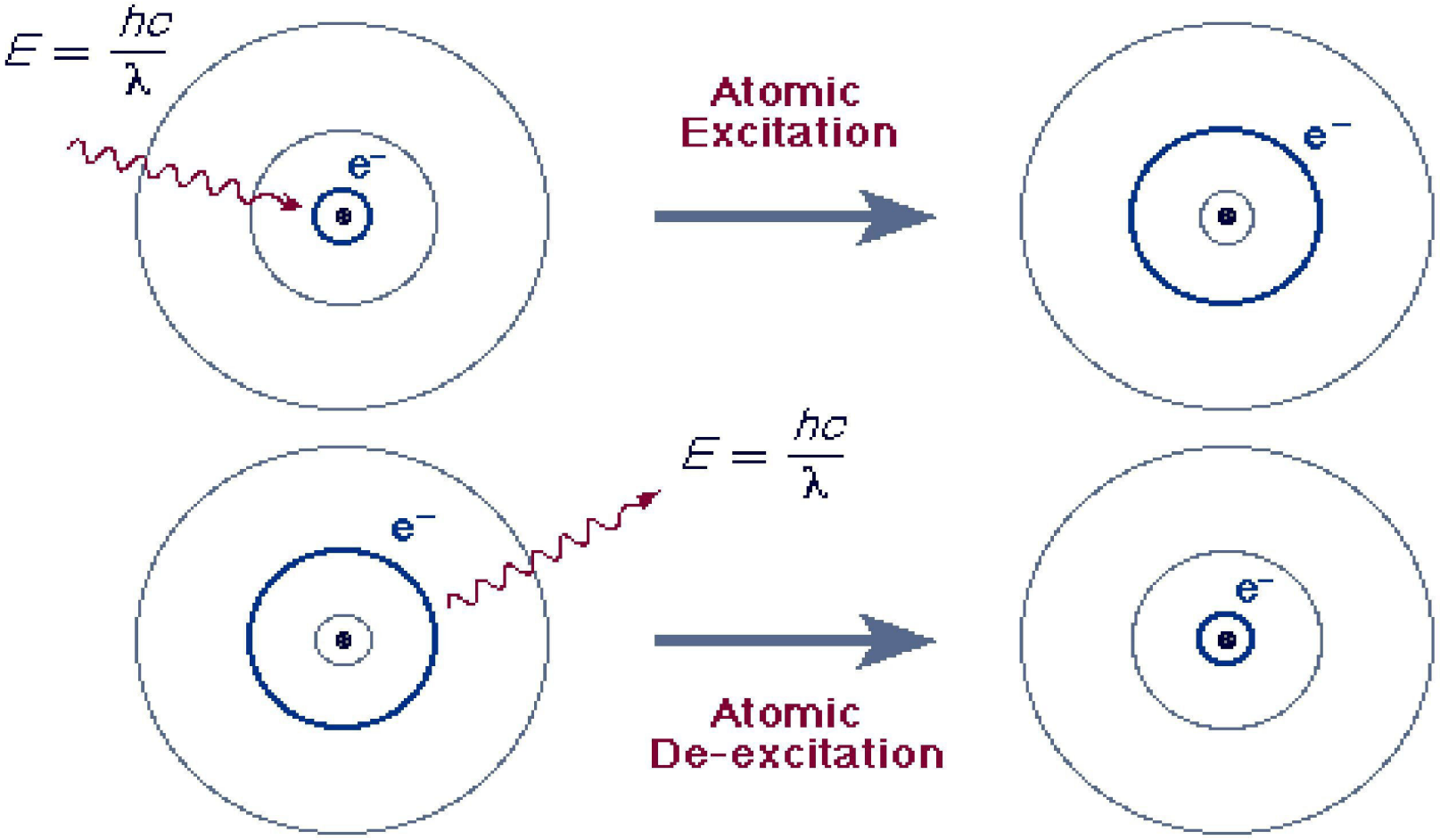


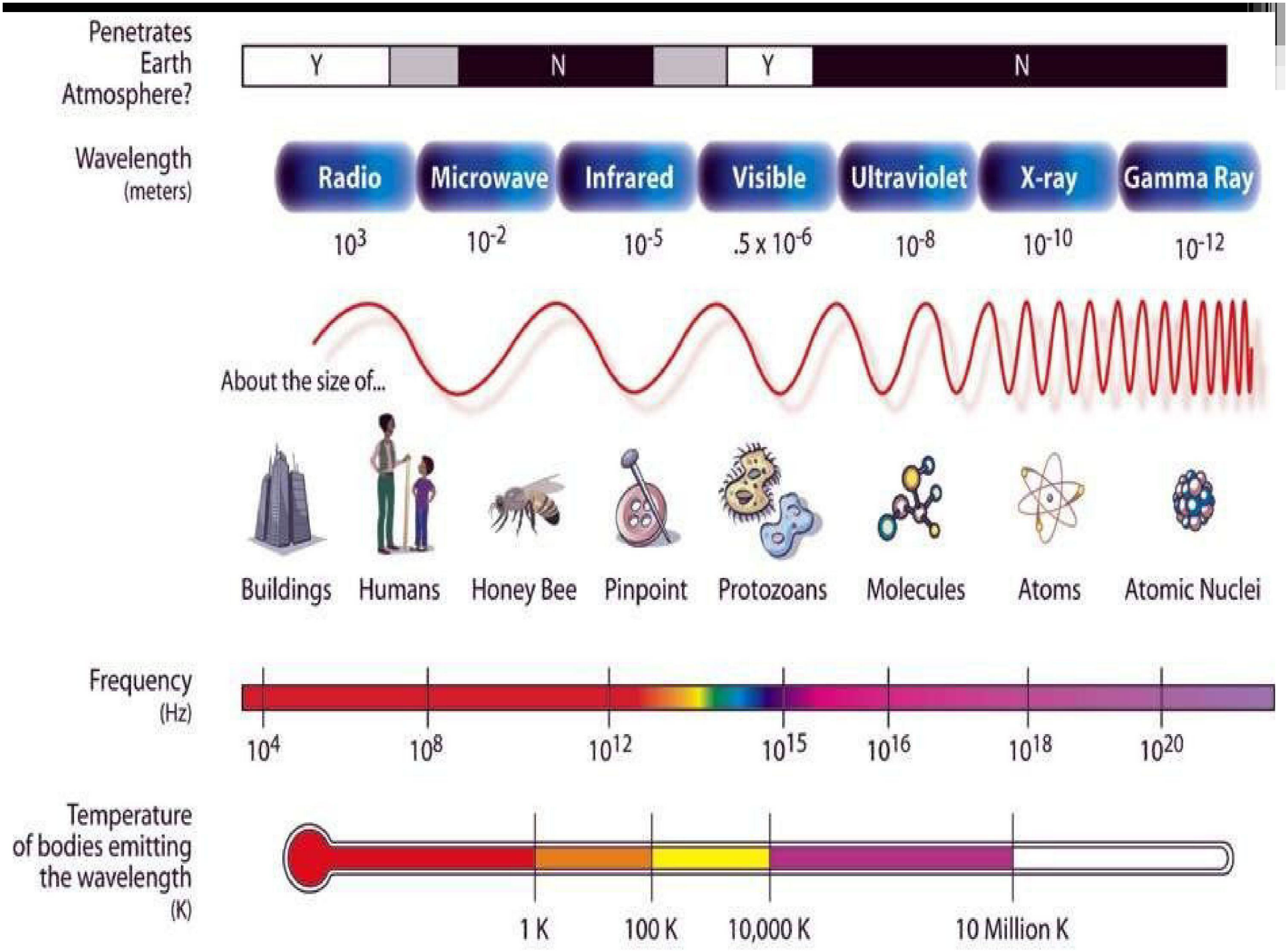


Innermost orbit is called as **K-shell.**
Followed by orbital's called **L-shell, M-shell** and **N-shell.**
The maximum no. of electrons in an orbital is given by the formula $\mathbf{2n^2}$**.**

Eg: 1) Hydrogen atom has 1 electron in K-shell
2)Helium atom has 2 electrons in K-shell
3)Oxygen atom has 8 electrons (2 in K-shell, 6 in L-shell)

The electrons in the atom can make transitions between the orbits allowed by quantum mechanics by absorbing or emitting exactly the energy difference between the orbits




Penetrates Earth Atmosphere?
Y
N
Y
N
Wavelength (meters)
Radio
Microwave
Infrared
Visible
Ultraviolet
X-ray
Gamma Ray
10^{3}
10^{-2}
10^{-5}
$.5 \times 10^{-6}$
10^{-8}
10^{-10}
10^{-12}
About the size of...
Buildings
Humans
Honey Bee
Pinpoint
Protozoans
Molecules
Atoms
Atomic Nuclei
Frequency (Hz)
10^{4}
10^{8}
10^{12}
10^{15}
10^{16}
10^{18}
10^{20}
Temperature of bodies emitting the wavelength (K)
1 K
100 K
10,000 K
10 Million K

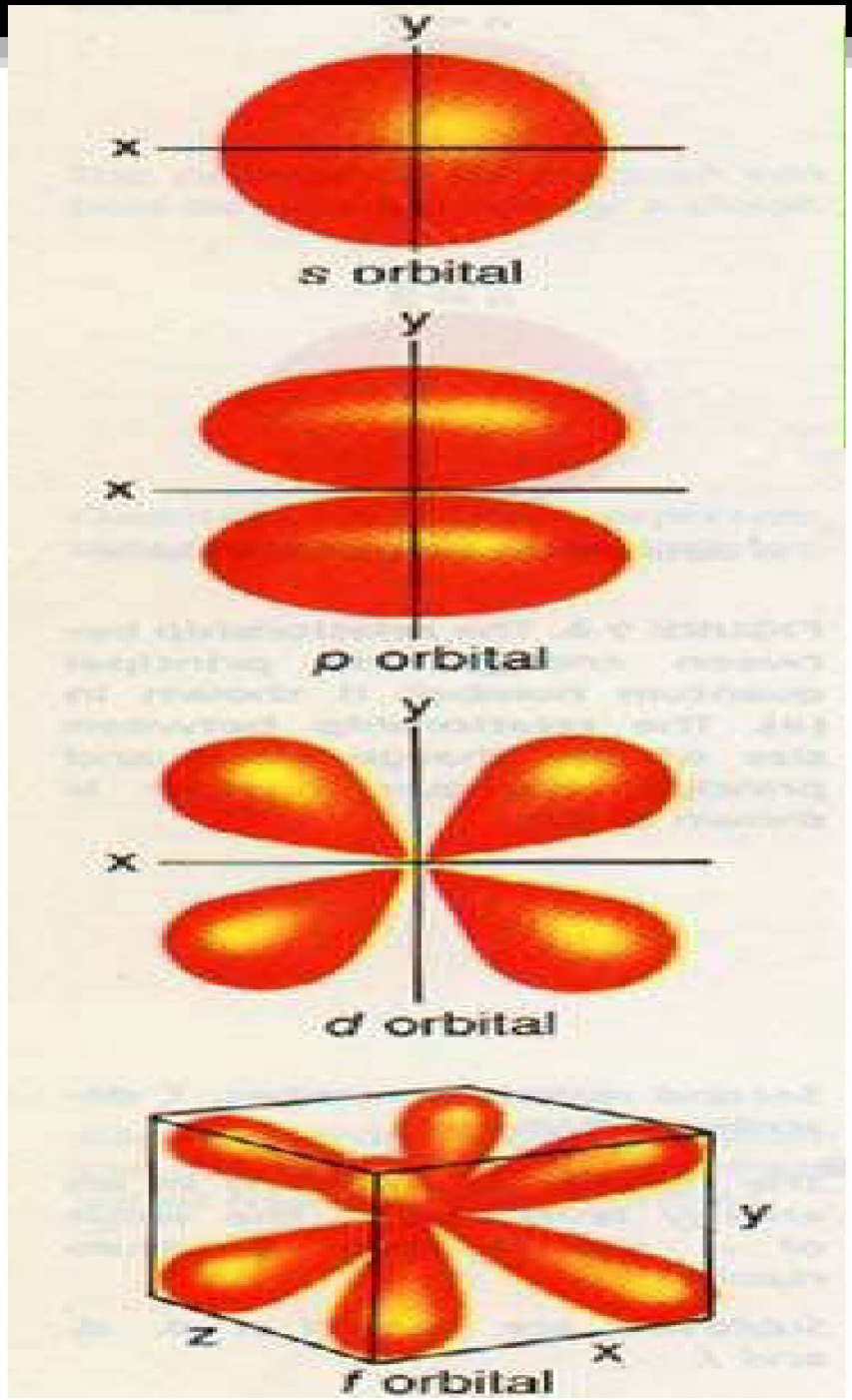
Quantum Numbers

- The Bohr model was a one-dimensional model that used one quantum number to describe the distribution of electrons in the atom.
- It therefore required four coordinates, or four **quantum numbers**, to describe the orbitals in which electrons can be found.
- the principal (n), angular (l), magnetic (m) and spin (s)quantum numbers. These quantum numbers describe the size, shape, orientation in space and spin of the orbitals on an atom.

- The **principal quantum number** (n) describes the size of the orbital. Orbitals for which $n = 2$ are larger than those for which $n = 1$, for example. The principal quantum number therefore indirectly describes the energy of an orbital.
- The **angular quantum number** (l) describes the shape of the orbital. Orbitals have shapes that are best described as spherical (s), two lobes (p), or complex (d and f).

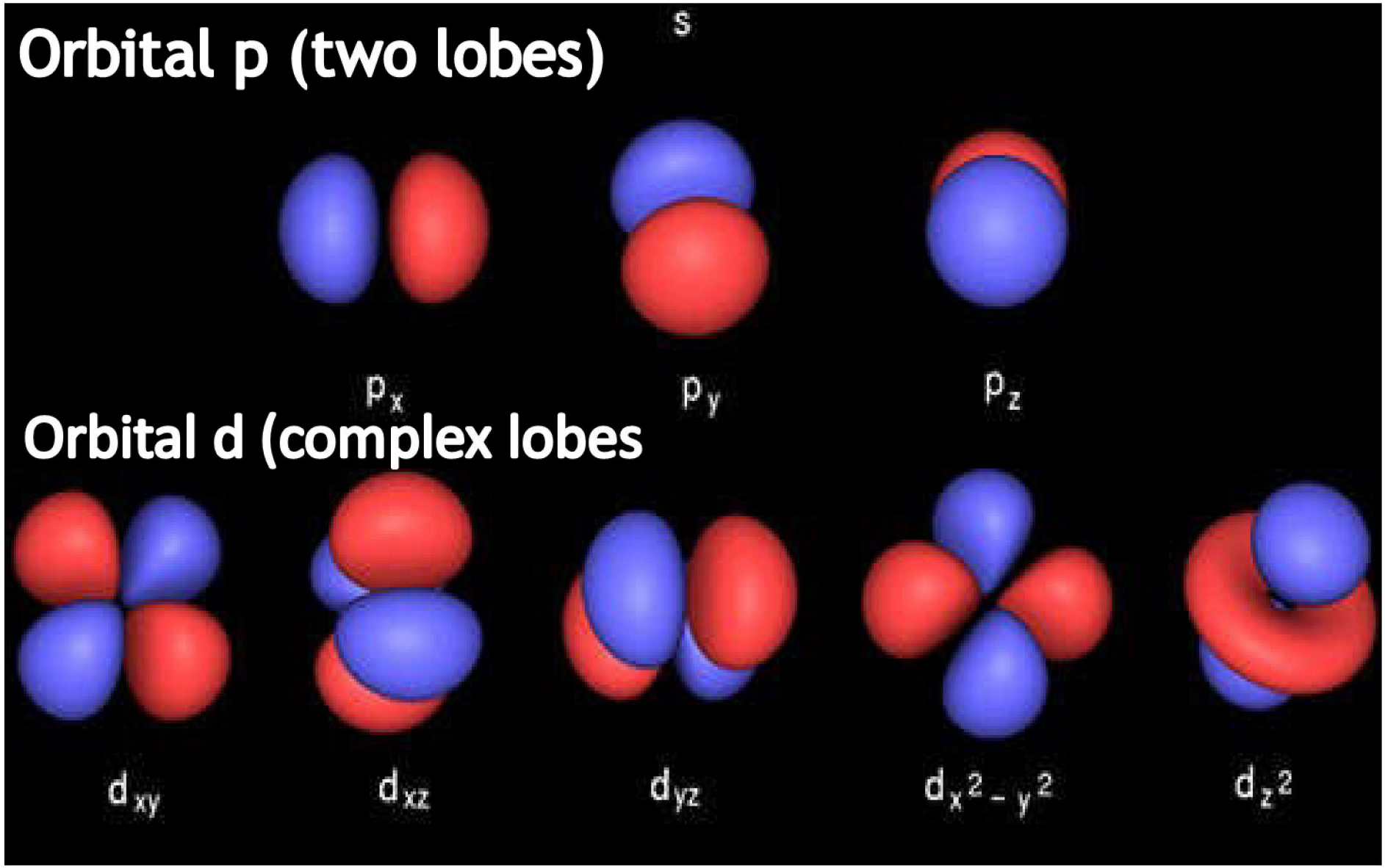
- The **magnetic quantum number** (m) describes the projection of the orbital angular momentum along a specified axis (x, y or z).

- The **spin quantum number** (s) describes the spin of the electron (-1/2 = counter-clockwise, 1/2 = clockwise).

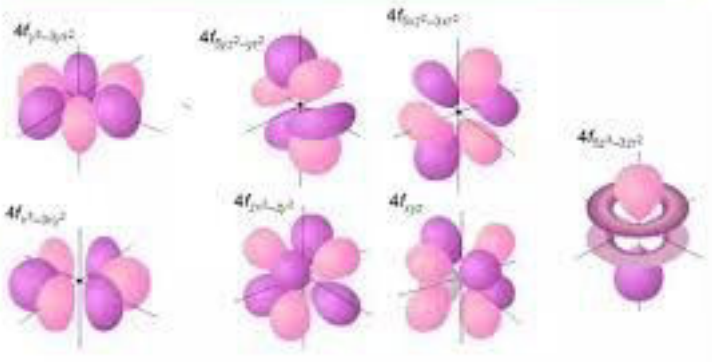


Quantum number l

Quantum number m

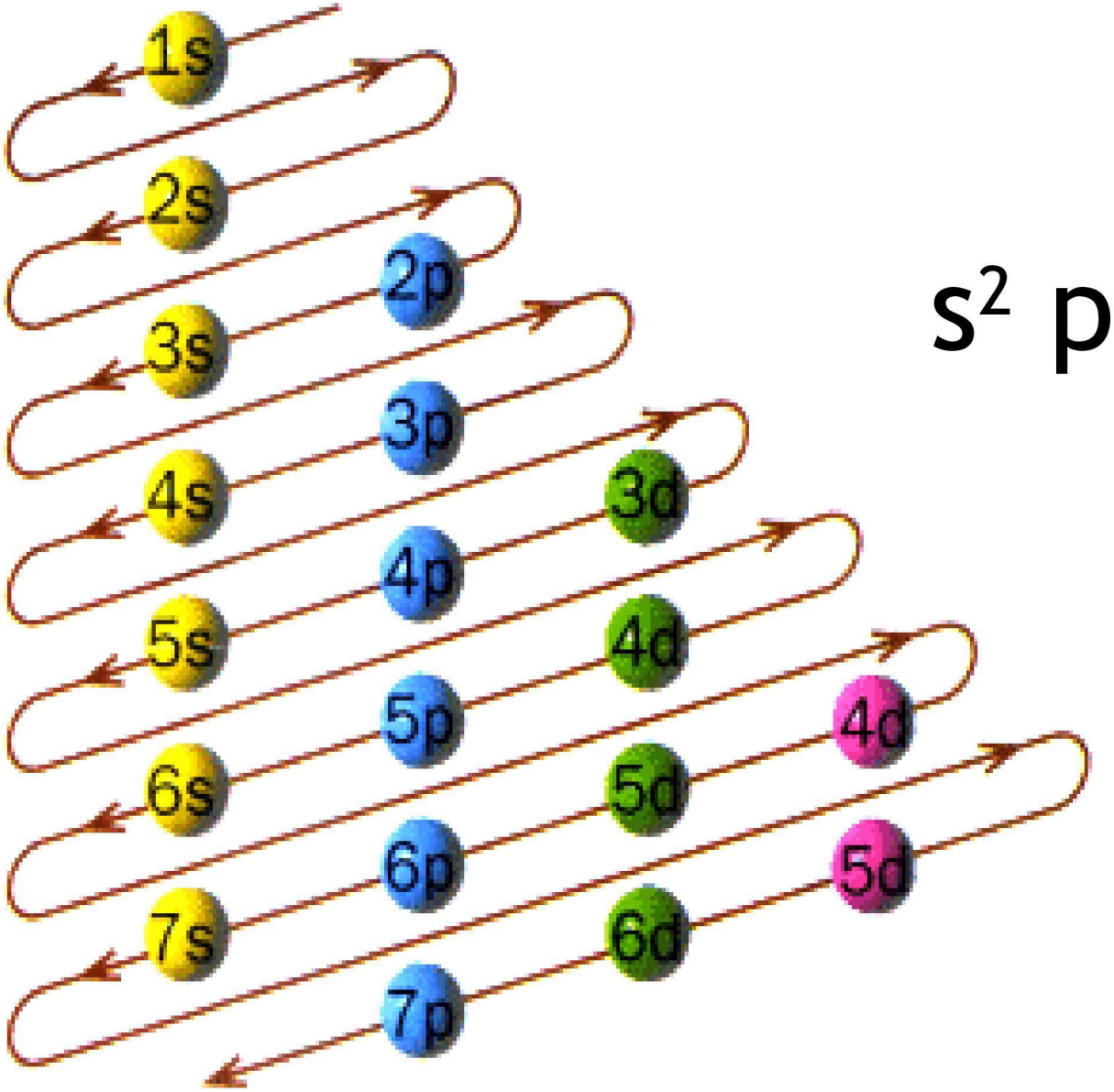


f orbitals



- **Orbital**: shows only the regions around the nucleus in which an electron has a relatively high probability of being found.
- **Pauli exclusion principle** : States that no more than two electrons (each with opposite spin ) can coexist in a single orbital.
- **Hund's Rule**: States that for the electrons in the same energy level have the tendency to occupy empty orbital avoiding overlapping with other electron.
- **The Aufbau Procedure**
- The aufbau procedure (filling order of atomic orbitals) is used to work out the electron confiturations of all atoms.

Hund's diagonal Rule



$s^2\ p^6\ d^{10}\ f^{14}$

Table 3-6a - Orbital and Electron Capacity for the Four Named Sublevels

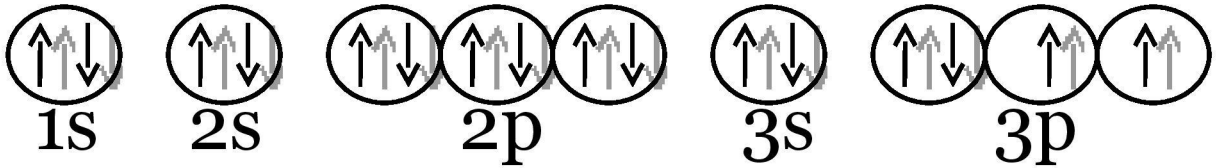
Sublevel	# of orbitals	Maximum number of electrons
s	1	2
p	3	6
d	5	10
f	7	14

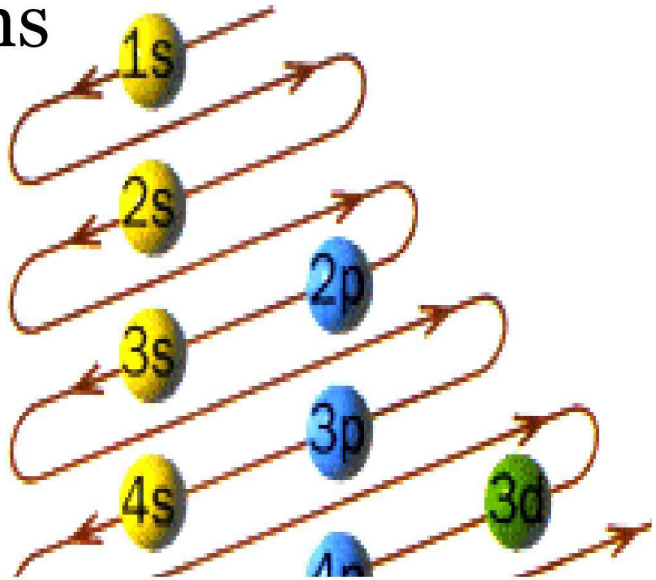
Table 3-6b Orbitals and Electron Capacity of the First Four Principle Energy Levels

Principle energy level (n)	Type of sublevel	Number of orbitals per type	Number of orbitals per level (n^2)	Maximum number of electrons ($2n^2$)
1	s	1	1	2
2	s	1	4	8
	p	3		
3	s	1	9	18
	p	3		
	d	5		
4	s	1	16	32
	p	3		
	d	5		
	f	7		

Example

- Sulfur Z=16 this means 16 electrons
- Use diagonal rule
- Electron's configuration diagram





- Electron's configuration

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$

*Check periodic table the energy level 3 is the period 3

And the position p the fourth place is sulfur

Applications Of Bohr's Atomic Model

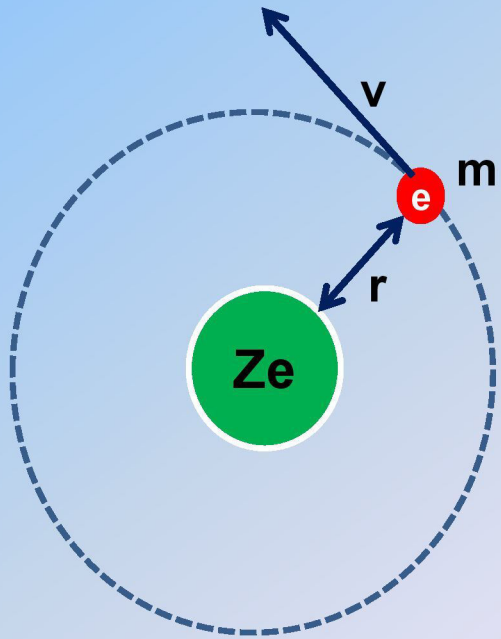
- Derivation of Radius of an Orbit of an atom
- Derivation of Energy of an Orbit
- Derivation of Wave Number ($\bar{u}$)

Prepared by: Sidra Javed

Derivation of Radius of an Orbit of an Atom

Consider an atom having an electron e^- moving around the nucleus having charge Ze where Z is the atomic number.

Let m be the mass, r the radius of the orbit and v, the velocity of the revolving electron.



According to Coloumb's law, the electrostatic force of attraction b/w nucleus and electron :

$$F_c = \frac{q_1 q_2}{4\pi\varepsilon_o r^2} = \frac{Ze.e}{4\pi\varepsilon_o r^2}$$

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

Where ε_o is the vacuum permittivity constant (ε_o = 8.84 x 10^{-12} $C^2/J.m$)

Centrifugal force acting on the electron = $\frac{mv^2}{r}$

The two forces are equal and balance each other

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

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

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

According to Bohr's postulate:

$$mvr = \frac{nh}{2\pi} \ldots\ldots\ldots\ldots\ldots(3)$$

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

$$v^2 = \frac{n^2h^2}{4\pi^2m^2r^2} \ldots\ldots\ldots(4)$$

Put value in eq(2).

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

$$\frac{1}{1} = \frac{Ze^2 \pi m r}{\varepsilon_\circ n^2 h^2}$$

$$Ze^2 \pi m r = \varepsilon_\circ n^2 h^2$$

$$r = \frac{\varepsilon_\circ n^2 h^2}{Ze^2 \pi m} \ldots\ldots\ldots\ldots\ldots (5)$$

For Hydrogen atom, Z = 1

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

$$r = \frac{\varepsilon_o n^2 h^2}{(1)e^2 \pi m}$$

$$r = \frac{\varepsilon_o n^2 h^2}{\pi m e^2} \ldots\ldots\ldots\ldots (6)$$

$$r = n^2 a^o$$

Where a^o is a constant quantity,

$$a^o = \frac{\varepsilon_\circ h^2}{e^2 \pi m}$$

$$a^o = 0.529 x 10^{-10} m$$

$$a^o = 0.529 \, \mathring{\mathrm{A}}$$

$$r = n^2 . a^o$$

So, $r = n^2 \times 0.529\,\text{Å}^{o}$

Therefore radius of orbits having n = 1, 2, 3… are as follows:

When n=1: $r_1 = (1)^2 \times 0.529 = 0.529\,\text{Å}^{o}$

When n=2: $r_2 = (2)^2 \times 0.529 = 2.11\,\text{Å}^{o}$

When n=3: $r_3 = (3)^2 \times 0.529 = 4.75\,\text{Å}^{o}$

When n=4: $r_4 = (4)^2 \times 0.529 = 8.4\,\text{Å}^{o}$

Derivation of Energy of an Electron in an Orbit

The energy of an electron in an orbit is the sum of its potential and kinetic energy

$$E_T = K.E + P.E$$

$$E_T = \frac{1}{2}mv^2 + \left(-\frac{Ze^2}{4\pi\varepsilon_o r}\right).....(7)$$

$$E_T = \frac{1}{2}mv^2 - \frac{Ze^2}{4\pi\varepsilon_o r}$$

From eq(1) $$mv^2 = \frac{Ze^2}{4\pi\varepsilon^\circ r}$$

Putting value in eq (7)

$$E_T = \frac{Ze^2}{2.4\pi\varepsilon^\circ r} - \frac{Ze^2}{4\pi\varepsilon^\circ r}$$

$$E_n = \frac{Ze^2}{8\pi\varepsilon_\circ r} - \frac{Ze^2}{4\pi\varepsilon_\circ r}$$

$$E_n = \frac{Ze^2}{4\pi\varepsilon_\circ r}\left(\frac{1}{2} - 1\right)$$

$$E_n = \frac{-Ze^2}{8\pi\varepsilon_\circ r} \ldots\ldots\ldots\ldots\ldots (8)$$

Now putting the value of *r* from eq(5) into eq(8),

$$E_n = \frac{-Ze^2}{8\pi\varepsilon_\circ} \times \frac{Ze^2\pi m}{\varepsilon_\circ n^2 h^2}$$

$$E_n = \frac{-Z^2 e^4 m}{8\varepsilon_o^2 n^2 h^2} \ldots\ldots\ldots\ldots (9)$$

For Hydrogen atom; Z=1

$$E_n = \frac{-me^4}{8\varepsilon_o^2 n^2 h^2}$$

$$E_n = -\frac{me^4}{8\varepsilon_o^2 h^2}\left[\frac{1}{n^2}\right]$$

But $$\frac{me^4}{8\varepsilon_o^2 h^2} = -2.178\times10^{-18}\,\mathrm{J}$$

$$E_n = -2.178\times10^{-18}\left(\frac{1}{n^2}\right)\mathrm{J}\ldots\ldots\ldots\ldots(10)$$

$$E_n = -\frac{k}{n^2}$$

$$\mathrm{where}\, k = 2.178\times10^{-18}$$

The negative sign indicated Decrease in energy of the electron.

For 1 mol of electron, multiply by Avogadro's No.

$$E_n = -\left(\frac{k}{n^2}\right) \times 6.02 \times 10^{23}\ \text{J/mol}$$

$$E_n = -\left(\frac{k}{n^2}\right) \times \frac{6.02 \times 10^{23}}{1000}\ \text{KJ/mol}$$

$$E_n = 1313.315\left(\frac{1}{n^2}\right)\text{KJ/mol}$$

This energy is associated with 1.008 gram-atoms of hydrogen.

If n=1, 2, 3,…. then;

$$E_1 = -1313.315\left(\frac{1^2}{1^2}\right) = -1313.315\,kJmol^{-1}$$

$$E_2 = -1313.315\left(\frac{1^2}{2^2}\right) = -328.32\,kJmol^{-1}$$

$$E_3 = -1313.315\left(\frac{1^2}{3^2}\right) = -145.92\,kJmol^{-1}$$

$$E_4 = -1313.315\left(\frac{1^2}{4^2}\right) = -82.08\,kJmol^{-1}$$

$$E_5 = -1313.315\left(\frac{1^2}{5^2}\right) = -52.53\,kJmol^{-1}$$

The first energy level when n=1 is called Ground state of H atom. All others are called Excited states.

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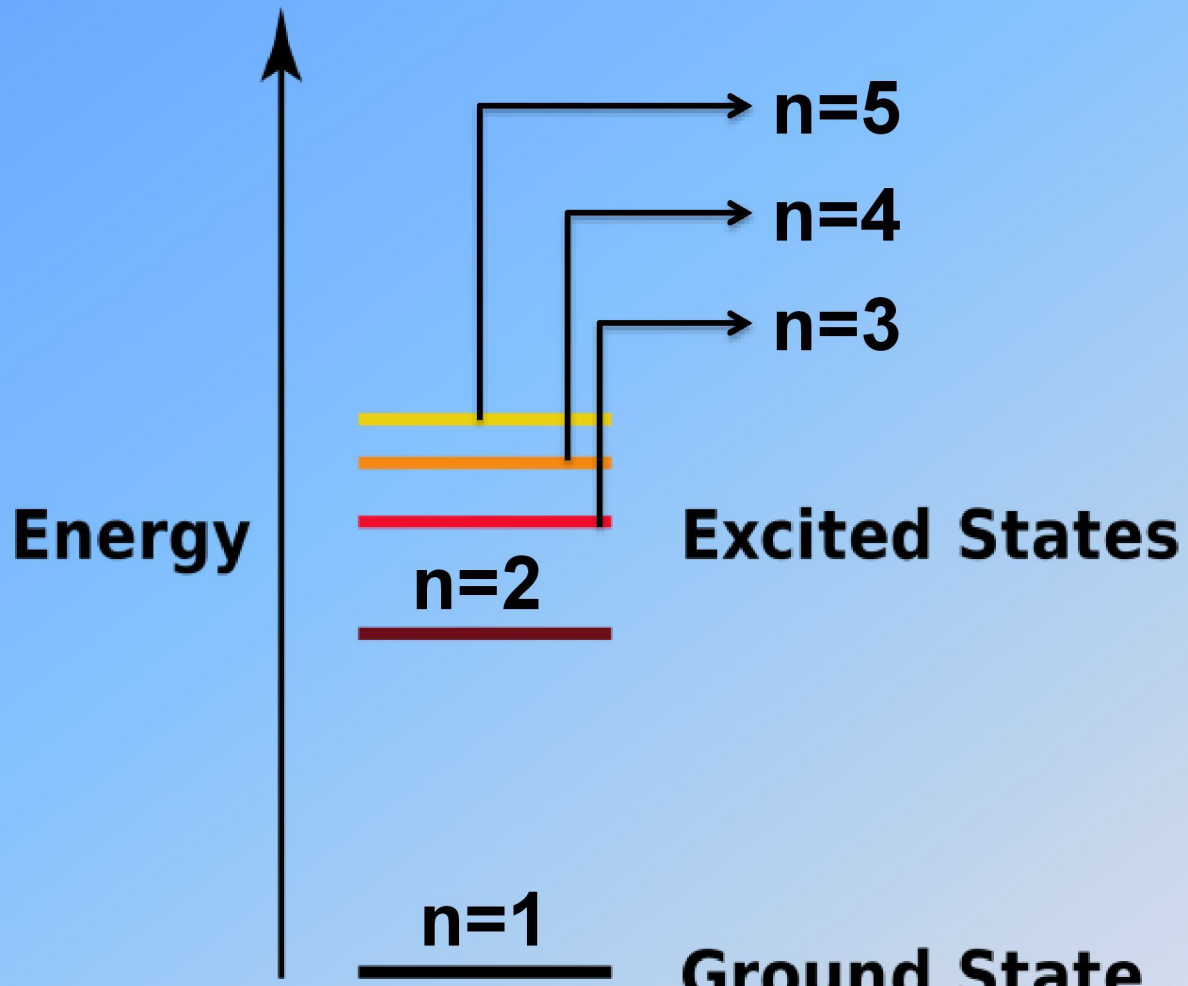

$E_5 = -52.53\ kJmol^{-1}$

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$E_2 = -328.32\ kJmol^{-1}$

$E_1 = -1313.315\ kJmol^{-1}$

Frequency of Radiation emitted by an Electron

From eq(9)

$$E_n = \frac{-Z^2 e^4 m}{8\varepsilon_o^2 n^2 h^2} \ldots\ldots\ldots\ldots (9)$$

Let,

E_1=energy of orbit n_1 $$E_1 = \frac{-Z^2 e^4 m}{8\varepsilon_o^2 n_1^2 h^2}$$

E_2=energy of orbit n_2 $$E_2 = \frac{-Z^2 e^4 m}{8\varepsilon_o^2 n_2^2 h^2}$$

$$\Delta E = E_2 - E_1$$

$$\Delta E = \frac{-Z^2 e^4 m}{8\varepsilon_o^2 n_2^2 h^2} - \left(\frac{-Z^2 e^4 m}{8\varepsilon_o^2 n_1^2 h^2} \right)$$

$$\Delta E = \frac{Z^2 e^4 m}{8\varepsilon_o^2 h^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

For H atom, Z=1

$$\Delta E = \frac{me^4}{8\varepsilon_o^2 h^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \ldots\ldots\ldots (11)$$

Here, $\frac{me^4}{8\varepsilon_o^2 h^2} = 2.18\times10^{-18}\,\text{J}$

$$\Delta E = 2.18\times10^{-18}\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)\ldots\ldots\ldots\ldots(12)$$

But according to Planck's Quantum Theory,

$$\Delta E = h\nu$$

$$\therefore h\nu = 2.18\times10^{-18}\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)$$

Again

$$h\nu = \frac{me^4}{8\varepsilon_o^2 h^2}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

or,

$$\nu = \frac{me^4}{8\varepsilon_o^2 h^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \text{Hz or Cycles.sec}^{-1} \ldots\ldots\ldots (3)$$

$$\nu = 3.29x10^{15}\left(\frac{1}{n_1^{\,2}} - \frac{1}{n_2^{\,2}}\right) \text{Hz}$$

Derivation of Wave number

$$\nu = c\bar{\upsilon} \ldots\ldots\ldots\ldots\ldots (14)$$

Where c is the velocity of Light

Putting value of ν from eq(13) into eq(14)

$$\bar{\upsilon}c = \frac{me^4}{8\varepsilon_o^2 h^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\bar{\upsilon} = \frac{me^4}{8\varepsilon_o^2 h^3 c}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \ldots\ldots\ldots\ldots\ldots (15)$$

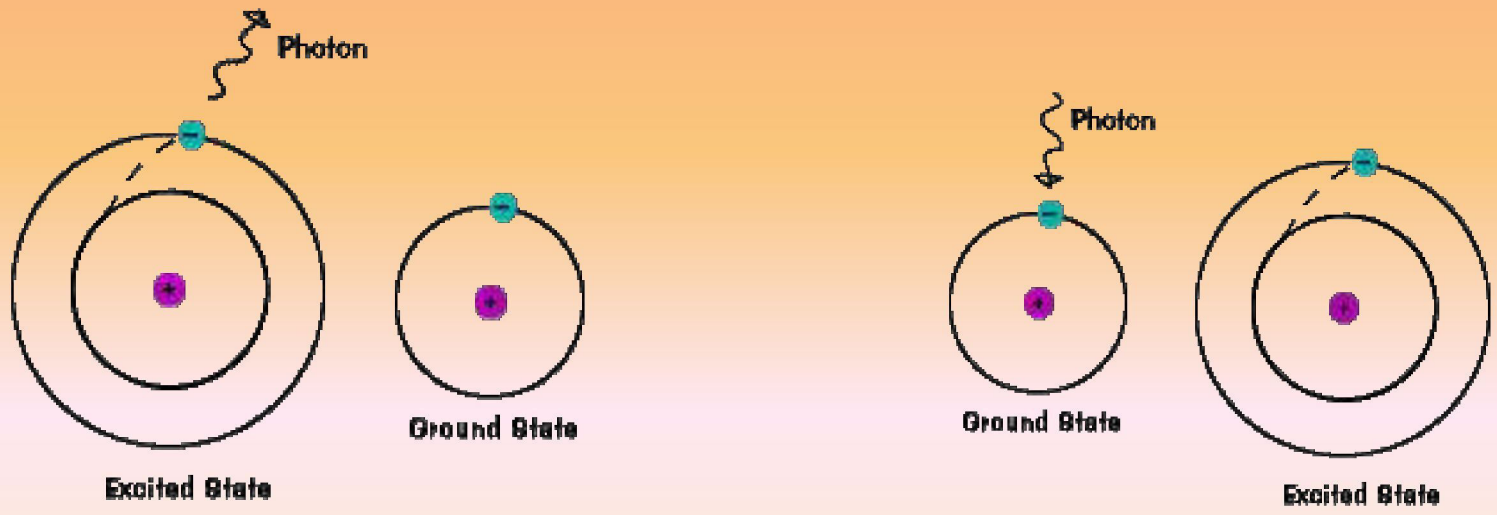
Putting values of constants, we get a factor called Rydberg's Constant, R.

$$\frac{me^4}{8\varepsilon_o^2 h^3 c} = R = 1.09678 \times 10^7 \,\mathrm{m}^{-1}$$

$$\therefore \bar{\upsilon} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \ldots\ldots\ldots\ldots\ldots (16)$$

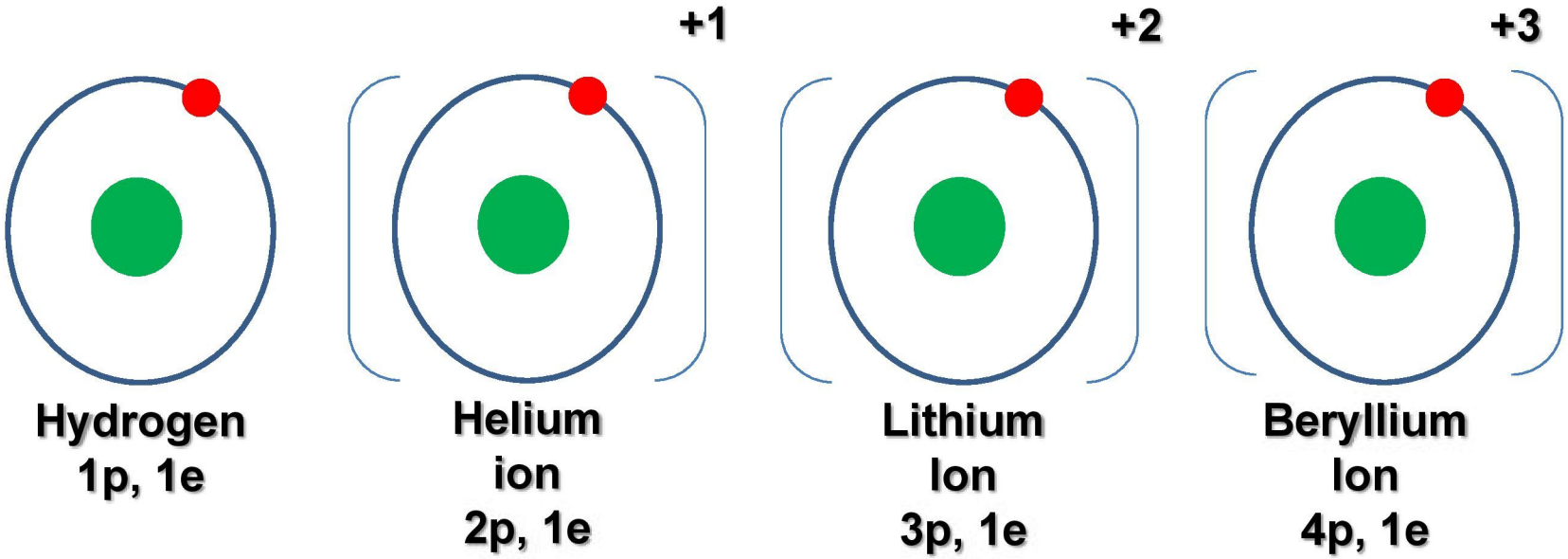
Defects of Bohr's Atomic Model

1- According to Bohr, the radiation results when an electron jumps from one energy orbit to another energy orbit, but he did not explained how this radiation occurs.



2- Bohr's theory explained the existence of various lines in H-spectrum, but it predicted that only a series of lines exist. Later on it was realized that the spectral lines that had been thought to be a single line was actually a collection of several lines very close to each other.

3- Bohr's theory successfully explained the observed spectra for H – atom and similar ions (He^{+1} , Li^{+2} , Be^{+3} etc) but it can not explained the spectra for poly electron atoms.



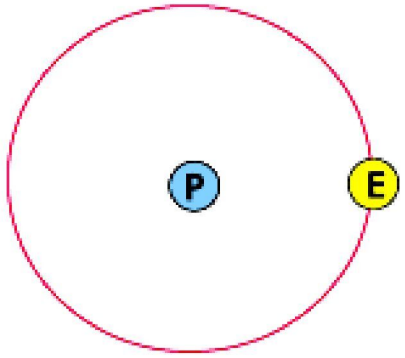
4- If a substance which gives line emission spectrum is placed in a magnetic field, the lines of the spectrum get split up into a number of closely spaced lines. This phenomenon is known as **Zeeman effect.** Bohr's theory has no explanation for this effect.

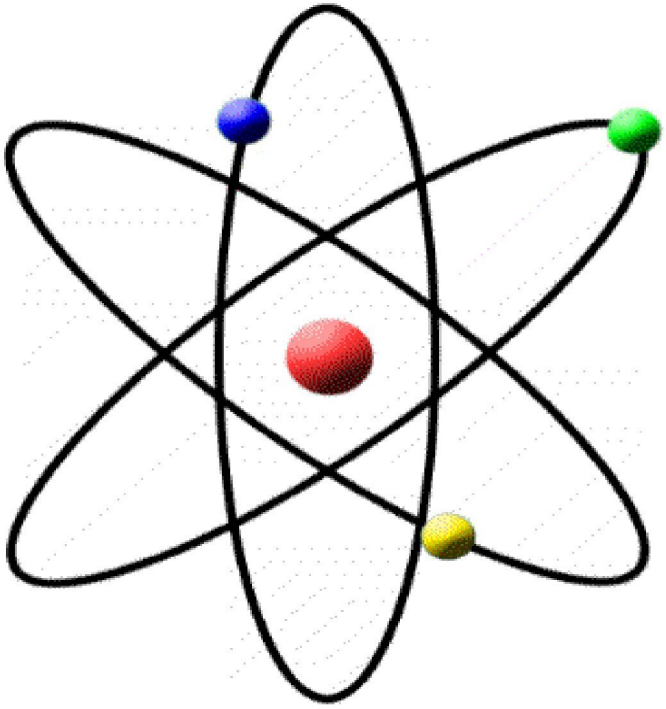
magnetic field
off

magnetic field
on

5- If a substance which gives line emission spectrum is placed in an external electric field, the lines of the spectrum get split up into a number of closely spaced lines. This phenomenon is known as **Stark effect.** Bohr's theory has no explanation for this effect as well.

6- Bohr suggested circular orbits of electron around the nucleus of H – atom but later it was proved that the motion of electron is not in a single plane, but takes place in three dimensional space.





7- Bohr's assumes that an electron in an atom is located at a definite distance from the nucleus and is revolving round it with definite velocity i.e. it has a fixed momentum.

This idea is not in agreement with **Heisenberg's uncertainty principle** which states that it is impossible to determine the exact position and momentum of a particle simultaneously with certainty.


The End
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