U-2

Structure of Atom

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- ~~It~~ Electron is just a wave which is moving around the nucleus in a fixed path.

Charge and mass of electron

Charge e^- = 1.6×10^{-19} ~~Culomb~~ Coulomb

Mass = 9.1×10^{-31} kg

Relative charge =

Proton

charge e^- = 1.6×10^{-19} C

Relative charge e^- = -1

Mass of proton M_p = 1.6×10^{-24} kg

Radioactivity

The phenomena of spontaneous emission of certain highly active radiation by radioactive substance.

Types of rays

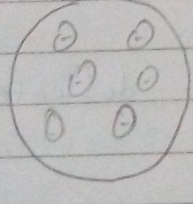
i) α - particle (same as He^{2+} particle)
Mass = 4u (6.6×10^{-24} g)
Charge = +2 (3.2×10^{-19} C)

ii) β - particle (same as e^-)
Mass = 9.1×10^{-31} kg
Charge = 1.6×10^{-19} C

iii) γ - particle (same as a photon)
light particle.
No charge
No mass

γ - particle has high penetrating power
α - particle is the heaviest

Thompson's model of atom.



+ve shell
-ve charges embedded in it

No. of +ve = No. of -ve charge

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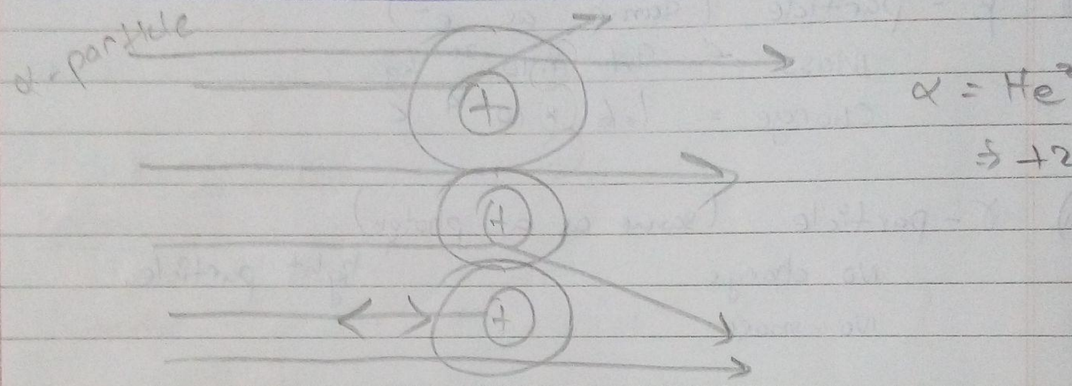
- Thompson's model of an atom can be visualised as a pudding or watermelon with a positively charged shell ~~and~~ with electrons embedded in it.

Rutherford's model ~~of~~ an atom



Rutherford's Gold foil experiment

The observation ~~from Ruther~~ :

i) Most of the alpha particle (about 99%) passed through the gold foil undeflected

ii) Some of the particles were deflected by small angles.

iii) A very few α-particles (1 out of 20k) suffered major deflection (more than 90°) and even came back in the same direction.

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Conclusion:

i) As most α-particle passed through the atom undeflected, thus most of the space inside an atom is empty.

ii) As a very few α-particle suffered minor deflection and a very few major deflection, this means that they must have came across some obstruction which is very small, dense and positively charged.

Rutherford regarded this small, heavy and positively charged portion as nucleus. The space surrounding the nucleus as extra-nuclear portion

Rutherford's model of atom.

i) An atom consists of two parts - nucleus and extra-nuclear portion.

ii) Nucleus is present in center of the atom. It is positively charged and extremely small.

iii) The positive charge of nucleus is due to protons.

iv) Extra-nuclear is ~~a~~ the space ~~in~~ around the nucleus in which electrons are present.

v) Total -ve charge on the nucleus = Total -ve charge on electrons as a whole the atom is neutral

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Electrons in extra-nuclear portion revolve around the nucleus at high speed in circular paths called orbit.

Neutrons are a neutral particle
Charge of n = 0
Mass of n = 1.6×10^{-24} g

Atomic number

(z) = No. of protons (p)

Mass number

(A) = No. of proton + no. of neutrons

$^{A}_{Z}H$ = $^{4}_{2}He$

Isotopes

Isotopes are the atoms of same element having same atomic number but different mass number.

H → $^{1}_{1}H$, $^{2}_{1}H$ (D) , $^{3}_{1}H$ (T)

Cl → $^{35}_{17}Cl$, $^{37}_{17}Cl$ | C = $^{12}_{6}C$, $^{13}_{6}C$, $^{14}_{6}C$

Isobars

Same mass number, different atomic number.

Eg.- $^{40}_{18}Ar$, $^{40}_{19}K$, $^{40}_{20}Ca$

Isotones

Atoms of different elements which have same no. of neutrons

$^{14}C \rightarrow P \rightarrow 6$, $n \rightarrow 8$

$^{15}N \rightarrow P \rightarrow 7$, $n \rightarrow 8$

$^{16}O \rightarrow P \rightarrow 8$, $n \rightarrow 8$

Q) The electronic configuration of M^{2+} is 2, 8, 14 and its atomic mass is 56. What is the no. of neutrons in the nucleus.

Sol $M^{2+} \rightarrow 2, 8, 14$

$M \rightarrow 2, 8, 16$

$\downarrow$

$A \rightarrow \cancel{28}$ 26

Atomic mass $\rightarrow$ 56

$\downarrow$

no. of p + no. of n

$\therefore$ No. of n = 56 - 26

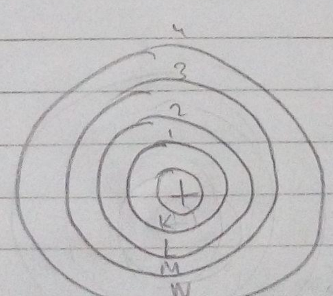
$\rightarrow$ 30

Failure of Rutherford's model of atom

⇒ According to Rutherford's model of atom the negatively charged electrons revolve around the positively charged nucleus. ~~We~~

We can say the electron is undergrowing acceleration. According to the radiation theory of Maxwell when a charged particle is accelerated it emit electro magnetic radiation. This means that revolving electron also lose energy continiously in the form of EM Radiation. The loss of energy brings the electron closer to the nucleus and ultimately fall into the nucleus following a spiral path. This means that atom must collapse, Rutherford couldn't counter the Maxwell's theory

~~A~~ Bohr's model of a Atom



Resonance stability

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It was primarily applicable to hydrogen and one electron species like ~~Ag~~ He^+ and Li^{2+}

i) In hydrogen atom electrons revolve around the nucleus in a well defined circular path of fixed radius and energy. The circular path is known as orbit and the corresponding energy state is called stationary state.

ii) The energy of an electron in ~~the~~ its orbit does not change on its own.

iii) When a required amount of energy is absorbed by the electron, it absorbs the same in fixed amounts of bundles. called quanta. and jumps to higher stationary state called excited state.

Mathematically

$$\Delta E = \underbrace{E_2}_{\text{Higher energy level}} - \underbrace{E_1}_{\text{Lower energy level}}$$

iv) Different energy level or energy shell for the electron are given as K, L, M, N or 1, 2, 3, 4

v) Only those energy orbits are permitted for the electron in which the angular momentum of the electron is a whole number multiple of $\frac{h}{2\pi}$ i.e.,

Plank's Constant

Rydberg's constant

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"$n \times \frac{h}{2\pi}$". Angular momentum of electron =
$\omega = mvr = \frac{nh}{2\pi}$ (h = plank's constant)

$$\boxed{h = 6.626 \times 10^{-34}}$$

vi) Energy of stationary state is given by

$$E_n = R_H\left(\frac{1}{n^2}\right)$$

$$\boxed{\begin{array}{l} R_H = \text{Rydberg's constant} \\ R_H = 2.18 \times 10^{-18}\ J \end{array}}$$

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Achievements of Bohr's Model

i) Bohr's theory has explained the stability of an atom.

ii) Bohr's theory has been used to derive Balmer's formula

$$E_f = R_H \left[\frac{1}{n_f^2}\right]$$

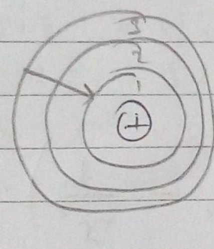
and

$$\Delta E = E_f - E_i$$

$$\Delta E = -\frac{R_H}{n_f^2} + \frac{R_H}{n_i^2}$$

$$\Delta E = \frac{R_H}{n_i^2} - \frac{R_H}{n_f^2}$$

$$\Delta E = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$



- If the electron moves from outer to inner shell, it releases energy in the form of EM waves

$$\Delta E = (2.18 \times 10^{-18}\ J) \left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) \quad J$$

The frequency for the absorbtion and emission of energy can be calculated as follows

Now,

$$\Delta E = h\nu$$

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

$$\Rightarrow \frac{2.18 \times 10^{-8}}{6.626 \times 10^{-34}} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$\nu = 3.29 \times 10^{15} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \text{ Hz or } s^{-1}$$

$$\bar{\nu} = \frac{\nu}{\text{speed of light}}$$

$$\Rightarrow \frac{3.29 \times 10^{15}}{3 \times 10^{8}} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$\bar{\nu} \Rightarrow 1.09677 \times 10^{7} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) m^{-1}$$

* Energy of electron in Hydrogen Atom.

Energy of n^{th} orbit is given by

$$E_n = \frac{-2\pi^2 k^2 m_e e^4 z^2}{n^2 h^2}$$

K = Permitivity of the

M_e = mass of e^-

e = charge of e^-

Z = nuclear charge

n = no. of e^- orbit

h = plank's constant

$$\boxed{E_n = \frac{-1312}{n^2} \text{ KJ mol}^{-1}}$$

For n = 1

E_1 = − 1312 kJ / mol

E_2 = − 328 kJ / mol

E_3 = − 145.8 kJ / mol

E_4 = − 82.0 kJ / mol

E_5 = − 52.5 kJ / mol

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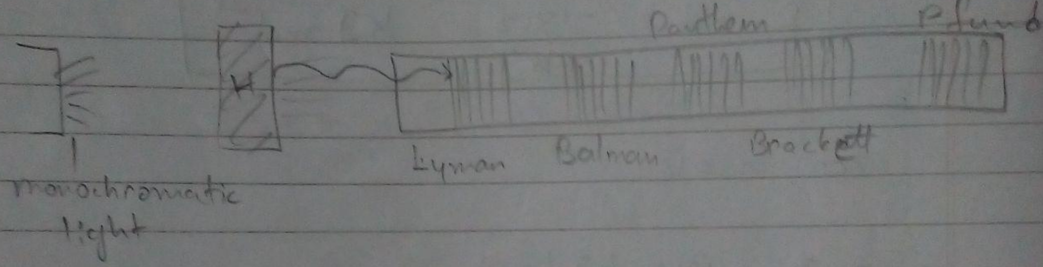
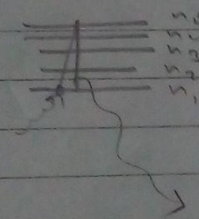
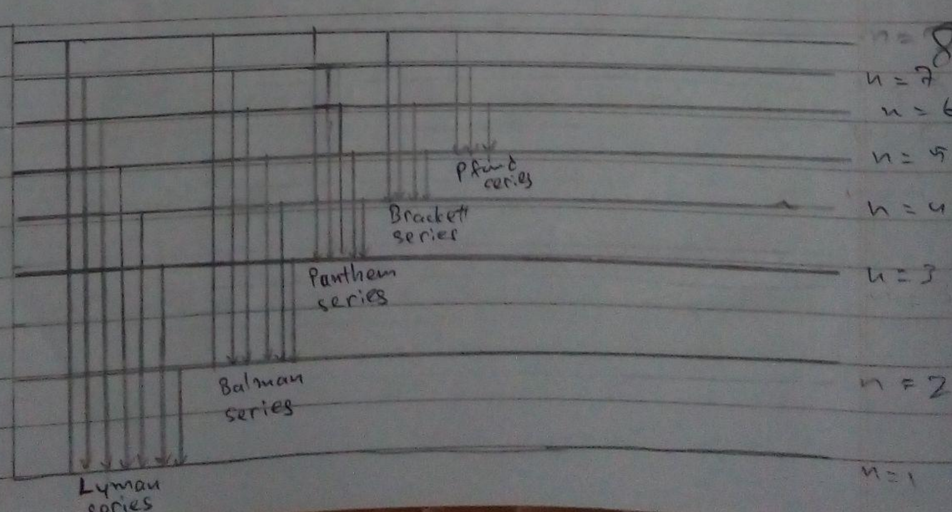
Explaination for the simultaneous appearance of many spectral light in hydrogen spectrum.

In study of hydrogen spectrum, the appearance of spectral lines in difference series of hydrogen spectrum such as





Spectral lines in different series of hydrogen spectrum.



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Q) In a hydrogen atom, an electron jumps from ~~first~~ third orbit to first orbit. Find out the frequency of spectral line.

$$\nu = 3.29 \times 10^{15} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$\Rightarrow 3.29 \times 10^{15} \left(\frac{1}{1^2} - \frac{1}{3^2} \right)$$

$$\Rightarrow 3.29 \times 10^{15} \left(\frac{9}{9} - \frac{1}{9} \right)$$

$$\Rightarrow 3.29 \times 10^{15} \times \frac{8}{9}$$

$$\Rightarrow \frac{27.32 \times 10^{15}}{9}$$

$$\Rightarrow 2.92 \times 10^{15} \text{ Hz}$$

Q) In a hydrogen atom, the energy of an electron in first Bohr's orbit is 13.12 × 10^5 J/mol. What is the energy required for its excitation to Bohr's second orbit.

$n = 1$

$E_1 = 13.12 \times 10^5$ J/mol

$$E_1 = \frac{2\pi^4 me^4}{(1)^2 h^2}$$

$n_2 = 2$

$$E_2 = \frac{2\pi^4 me^4}{(2)^2 h^2}$$

$$\Rightarrow \frac{\cancel{13.12} \times 10^5}{\cancel{4}} \quad \cancel{6.56} \quad 3.28 \quad \Rightarrow 3.28 \times 10^5 \text{ J/mol}$$

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Q) In a hydrogen atom, an electron jumps from ~~first~~ third orbit to first orbit. Find out the frequency of spectral line.

$$\nu = 3.29 \times 10^{15} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$\Rightarrow 3.29 \times 10^{15} \left(\frac{1}{1^2} - \frac{1}{3^2} \right)$$

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$$E_2 = \frac{2\pi^4 me^4}{(2)^2 h^2}$$

$$\Rightarrow \frac{\cancel{13.12}^{\cancel{6.56}\ 3.28} \times 10^5}{\cancel{4}\ \cancel{2}} \Rightarrow 3.28 \times 10^5 \text{ J/mol}$$

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- Wavelength is inversely proportional to energy.

$\Delta E = (3.28 \times 10^{5}) - (13.12 \times 10^{5})$

$\Rightarrow -9.84 \times 10^{5}$

Q5) What are the two longest wavelength lines (in nanometer) in Lyman series of Hydrogen atom.

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

$\frac{1}{\lambda} = \frac{1.0967 \times 10^{7}}{\cancel{\quad}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) nm^{-1}$

for n=3 $\frac{1}{\lambda} = \frac{1.0967 \times 10^{7}}{10^{-9}} \left(\frac{1}{1^2} - \frac{1}{3^2} \right) nm^{-}$

$\Rightarrow \cancel{\ } 1.0967 \times 10^{-2} \times \frac{8}{9}$

$\lambda \Rightarrow \frac{9}{1.0967 \times 10^{-2} \times 8}$

$\Rightarrow \frac{9}{8.7736 \times 10^{-2}}$ ~~m~~ nano meter.

$\Rightarrow 121.54$ nm

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For $n=2$

$$\frac{1}{\lambda} = \frac{1.0967 \times 10^{7}}{10^{9}} \left(\frac{1}{1^2} - \frac{1}{2^2} \right) nm^{-1}$$

$$\Rightarrow 1.0967 \times 10^{-2} \left(\frac{1}{1} - \frac{1}{4} \right) nm$$

$$\Rightarrow 1.0967 \times 10^{-2} \times \frac{3}{4} \quad nm$$

$$\lambda = \frac{4}{1.0967 \times 10^{-2} \times 3}$$

$$\Rightarrow \frac{4}{3.2901 \times 10^{-2}}$$

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Limitations of Bohr's model:

i) The theory could not explain the atomic spectra of the atoms containing more than one electron.

ii) Bohr theory predicted only one spectral line for electronic transistion between two energy level. However if examined carefully, certain single lines found to contain

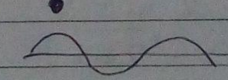
iii) a number of fine lines.

iii) The splitting of lines in the magnetic field is known as Zeeman effect and in the electric field is called Stark effect. When the source emitting this radiation is subjected to magnetic or electric field, each spectral line is found to split in number of lines.

iv) It cannot explain the shape of the molecule.

v) The theory also failed to explain new principles such as de-Broglie relationship and Heisenberg Uncertainity Principle.

Dual Behavior of Matter (De-Broglie's equation)

2 nature
↳ Particle $e^- \rightarrow$ •
↳ Wave $e^- \rightarrow$ 

• ~~For~~ All moving particle (microscopic as well as macroscopic) have dual nature, i.e., wave and particle nature.

De-Broglie's eq^n :-

$$\boxed{\lambda = \frac{h}{p}}$$, p = momentum of the particle
λ = wavelength ~~of the particle~~
h = Planck's constant
$h = 6.626 \times 10^{-34}$ kg m^2/s

Also $\Rightarrow$ $\boxed{\lambda = \frac{h}{mv}}$

$$\boxed{\text{wave nature} \propto \frac{1}{\text{Particle nature}}}$$

Relationship between De-Broglie eq^n and kinetic energy

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

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

Multiplying 2m on both side

$$2mE = 2m \times \frac{1}{2} v^2$$

$$2mE = m^2v^2$$
$$\sqrt{2mE} = P$$

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

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

Q) Find the wavelength of a 100 g particle moving with a velocity of 100 m/s.

Sol

$$\lambda = \frac{6.626 \times 10^{-34} \cancel{kg}\ m^2/s}{0.1\ \cancel{kg} \times 100\ \cancel{m/s}}$$

$$\frac{100}{1000}$$

$$\Rightarrow 6.626 \times \frac{1}{10} \times 10^{-34} \Rightarrow 6.626 \times 10^{-35}\ m$$

Q) Calculate the mass of photon of Na light having wavelength 5894 Å and velocity 3×10^8 m/s.

Sol

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

$$5894 \times 10^{-10} = \frac{6.626 \times 10^{-34}\ kg\ m^2/\cancel{s}}{m \times 3 \times 10^8\ m/\cancel{s}}$$

$$m = \frac{6.626 \times 10^{-34}}{3 \times 10^8 \times 5894 \times 10^{-10}}\ kg$$

$$\Rightarrow \frac{6.626 \times 10^{-24}}{3 \times 10^8}$$

$$\Rightarrow \frac{6.626 \times 10^{-32}}{3} \Rightarrow 2.2086 \times 10^{-32}\ kg$$

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Q) Calculate the De-Broglie wavelength of an electron moving with 1% of the speed of light.

Sol) mass of electron = 9.1×10^{-31} kg

$$\lambda = \frac{6.626 \times 10^{-34} \ \cancel{kg} \ m^2/\cancel{s}}{9.1 \times 10^{-31} \ \cancel{kg} \times 3 \times 10^8 \times \frac{1}{100} \ \cancel{m/s}}$$

$$\Rightarrow \frac{6.626 \times 10^{-34} \ m}{9.1 \times 10^{-31} \times 3 \times 10^6}$$

$$\Rightarrow \frac{6.626 \times 10^{-9} \ m}{9.1}$$

$$\Rightarrow 7.2 \times 10^{-10} \ m$$

Q) The kinetic energy of an electron is 4.55×10^{-25} Joule. The mass of electron is 9.1×10^{-31} kg. Calculate velocity, momentum and wavelength of the electron.

Sol) $K.E. = \frac{1}{2} m v^2$

$p = mv$

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

$K.E. = \frac{1}{2} m v^2$

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

$v^2 = \dfrac{\overset{1}{\cancel{4.55}} \times 10^{-25}}{\cancel{4.55} \times 10^{-31}}$ $\qquad \frac{25}{\frac{31}{14}}$

$\Rightarrow 10^{6}$ $\qquad \frac{31}{25}$

$v = \sqrt{10^6}$

$\Rightarrow 10^{3}$ m/s

$p = 9.1 \times 10^{-31} kg \times 10^{3}$ m/s

$\Rightarrow 9.1 \times 10^{-28}$ kg m/s

$\cancel{3.313}$ $\cancel{1.656}$ $\cancel{0.828}$ $\cancel{0.414}$

$\lambda = \dfrac{6.626 \text{ kg m}^2/\text{s}}{\cancel{9.1} \times 10^{-28} \text{ kg m/s}}$ $\qquad \cancel{0.207}$ $\qquad 0.7$ $\qquad \cancel{0.69}$ $\cancel{0.23}$

$\cancel{4.55}$ $\cancel{2.27}$

$\cancel{1.13}$ $\cancel{0.55}$ $\cancel{0.27}$ $\cancel{0.1}$ $\cancel{0.3}$ 0.1

$\Rightarrow 0.07 \times 10^{28}$

$\Rightarrow 7 \times 10^{30}$

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Q) What is the wavelength for the electron accelerated by 1×10^4 volts.

Sol ~~E = 10~~ $KE = 10^4 \times 1.6 \times 10^{-19}$

$\Rightarrow 1.6 \times 10^{-15}$ J

$KE = \frac{1}{2} \times m v^2$

$1.6 \times 10^{-15} = \frac{1}{2} \times \overset{4.55}{\cancel{9.1}} \times 10^{-31} \times v^2$

$\cancel{0.8}$ $\cancel{0.4}$ $\cancel{0.2}$ 0.1

$v^2 = \dfrac{\cancel{1.6} \times 10^{-15}}{\cancel{2.27}\ \cancel{4.55} \times 10^{-31}}$

$\cancel{1.13}$ $\cancel{0.56}$ 0.28

$\Rightarrow \dfrac{10^{16}}{0.28}$

$\Rightarrow 3.06 \times 10^{18}$

$v = 1.74 \times 10^{9}$ m/s

$\lambda = \underline{6.626 \text{ kg m}^2/\text{s}}$

$\frac{2\,11}{31}$
$\frac{15}{16}$

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1 pm = 10^{-12} m

Q) Calculate the kinetic energy of a moving electron which has the wavelength of 4.8 picometre.

Sol

$\lambda = 4.8 \times 10^{-12}$ m

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

$4.8 \times 10^{-12}\ m = \frac{6.626 \times 10^{-34}\ kg\ m^2/s}{9.1 \times 10^{-31}\ kg \times v}$

$v = \frac{6.626 \times 10^{-34}}{9.1 \times 10^{-31} \times 4.8 \times 10^{-12}}$

$\Rightarrow 0.151 \times 10^{9}$ m/s

$\Rightarrow 1.52 \times 10^{8}$ m/s

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

$\Rightarrow \frac{1}{2} \times 9.1 \times 10^{-31} \times (1.52 \times 10^{8})^2$

$\Rightarrow \frac{1}{2} \times 9.1 \times 10^{-31} \times 2.31 \times 10^{16}$

$\Rightarrow 1.051 \times 10^{-14}$ J

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Q) When would wavelength associated with an electron become equal to the wavelength associated with a proton. Given $M_e = 9.10 \times 10^{-28}$ g

$M_p = 1.67 \times 10^{-24}$ g

Sol

$\lambda_e = \frac{h}{m_e v_e}$

$\lambda_p = \frac{h}{m_p v_p}$

$\lambda_e = \lambda_p$

$\frac{\cancel{h}}{m_e v_e} = \frac{\cancel{h}}{m_p v_p}$

$\frac{m_p}{m_e} = \frac{v_e}{v_p}$

$\frac{v_e}{v_p} = \frac{1.67 \times 10^{-24}}{9.10 \times 10^{-28}}$

$\Rightarrow 0.1835 \times 10^{3}$

$\Rightarrow 183.5$

∴ The wavelengths will be equal when the velocity of electron is 183.5 times the velocity of proton.

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Heisenberg's Uncertainity Principle

It is not possible to measure simultaneously the position and the momentum of a microscopic particle with absolute accuracy or certainity.

Alternatively, the product of uncertainity in position and uncertainity in momentum of a microscopic particle is always constant and ~~gree~~ greater than or equal to $h/4\pi$.

Mathematically

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

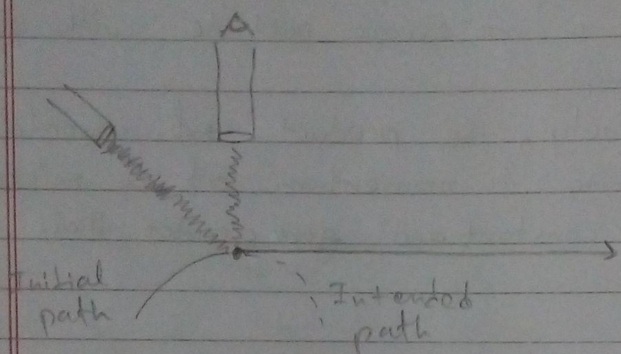
Significance of Heisenberg's Uncertainity Principle

According to the principle of optics, the accuracy with ~~which~~ which a particle can be located depends upon the wavelength of the light used. The uncertainity in position is $\pm \lambda$

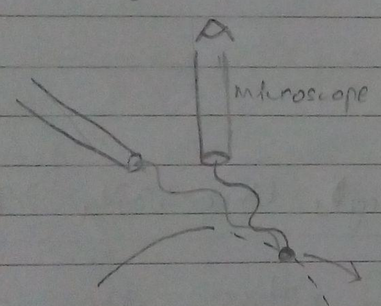
$$\uparrow E = \frac{hc}{\lambda \downarrow}$$

More the energy, lower the wavelength.

We cannot see a microscopic particle like electron without disturbing it.



High energy



Low energy

Q> A microscope using suitable photons is employed to locate an electron in an atom within a distance of 0.1 Å. What is the uncertainity involved in the measurement of its velocity?

$\Delta x = 0.1$ Å $= 0.1 \times 10^{-10}$ m

$\Delta v = ?$

$$\Delta x \, \Delta p = \frac{h}{4\pi}$$

$$\Delta x \, \Delta(mv) = \frac{h}{4\pi}$$

$$\Delta x m \, \Delta v = \frac{h}{4\pi}$$

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

$$\Delta v \geq \frac{6.626 \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.1 \times 10^{-10}}$$

$$\Delta v \geq 5.79 \times 10^{6} \text{ m/s}$$

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Q) A golf ball has mass of 40 g and speed of 45 m/s. If the speed can be measured within an accuracy of 2%. calculate the uncertainity in its position.

S) $m = 40\,g = 0.04\,kg$

$v = 45\,m/s$

$\Delta v = 2\%$ of 45

$\Delta x = ?$

$$\Delta x \geq \frac{6.626 \times 10^{-34}}{4 \times 3.14 \times 0.04 \times 0.9}$$

$$\Delta x \geq 1.465 \times 10^{-33}\ m$$

Q) A proton is accelerated to $\frac{1}{10}$ of velocity of light. If the ~~v~~ velocity can be measured with a precision of 0.5% what must be the uncertainity in its position?

Sol
$$\Delta x = \frac{h}{4\pi m \Delta v}$$

$$\Delta v = \frac{c}{10} = 3 \times 10^{7} \text{ m}$$

$$\Delta x = \frac{\cancel{6.626}^{3.313} \times 10^{-34}}{2\,\cancel{4} \times 3.14 \times 1.672 \times 10^{-27} \times \cancel{2}^{3} \times 10^{7}}$$

$$\Rightarrow \cancel{1.5}\ 1.05 \times 10^{-13} \text{ m}$$

Q) The uncertainity in measuring the speed of an accelerated electron is 1.2×10^{5} m/s. Calculate the uncertainity in finding its location while it is still in motion.

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

$$\Rightarrow \frac{\cancel{6.626}^{3.313} \times 10^{-34}}{4 \times \cancel{3.14} \times 9.1 \times 10^{-28} \times 1.2 \times 10^{5}}$$

1.57

$$\Rightarrow \frac{3.313 \times 10^{-11}}{44.68}$$

$$\Rightarrow 4.7 \times 10^{-11} \text{ m}$$

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Quantum Mechanical Model of Atom

Schrödinger wave equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}\left[E - V\right]\psi = 0$$

Where x, y, z are space coordinates

m = mass of e^-

E = Total energy of e^-

V = Potential energy

$\frac{d}{dx}$ – complete derivati[on]

$\frac{\partial}{\partial x}$ – partial derivation

ψ = (Psi) Wave function or Eigen function

- The atomic model developed Erwin Schrödinger have taken into account both wave and particle nature of the electron. It describes the electron as a three dimentional wave in the electronic field of positively charged nucleus.

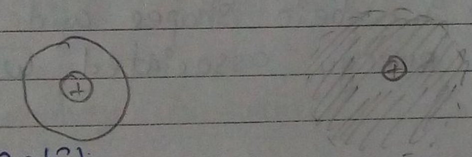
$|\psi|^2$ = Probability

Important Consequences of Quantum Mechanical Model of Atom

1. The energy of electrons in an atom is quantized, i.e., it can have only certain specific values

2. The quantized energy levels in which electrons can be present are obtained from the solution of Schrödinger equation.

3. As pointed by Heisenberg's Uncertainity Principle both position and velocity of electron cannot be determined simultaneously. The path of electron is only probable. This had led to ~~to~~ the concept of Atomic orbital.



orbit

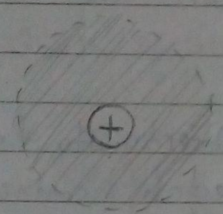
Orbital

4. In each orbital, ~~of~~ the electron has a definite energy and cannot have more than two electrons

5. The probability of finding an electron at a point within an atom is proportional to the square of wave function. It is also known as probability density. Finding the electron in the region near the ~~6. Fin~~ nucleus will be most probable.

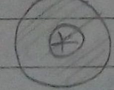
Atomic Orbitals and Quantum Numbers-

~~The region~~ Orbitals can be defined as the region in the space around the nucleus where the probality of finding the electron is maxium



Atomic orbital

>>> The orbitals differ in their shapes and sizes depending upon the energy associated with them



S- orbital

P- Orbital

D- orbital

Q) Write the differences between orbit and orbital.

s) Orbit : An orbit refers to the path followed by an electron around the nucleus of an atom. This concept is based on Bohr model of the atom, which suggests that electrons move in specific circular orbits at fixed distances from the nucleus.

Orbitals : Orbitals are regions of space around the nucleus where electrons are likely to be found. They do not have a defined path, instead, they describe the probability distribution of finding an electron in a particular region.

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Quantum Numbers

A set of four numbers which gives a complete information about the electron in an atom, i.e., its energy, shape, orientation and also its spin.

1. Principle Quantum Number (n) : It determines the main energy level or shell in which an electron in an atom is present and also the energy associated with it. The maximum number of electron that a shell can accomodate is given by $2n^2$, where $n = 1, 2, 3, 4 \ldots$

For $n = 2$, $2 \times (2)^2 = 8$

2. Angular Quantum Number (l) : Based on the energy ~~number~~ of electron the shells are devided into sub-levels or sub-shells. The value of 'l' can range from 0 to (n-1).

Value of n	value of l	Name of subshell
For n = 1,	$l = 0$	1s
For n = 2,	$l = 0, 1$	2s, 2p
For n = 3,	$l = 0, 1, 2$	3s, 3p, 3d
For n = 4	$l = 0, 1, 2, 3$	4s, 4p, 4d, 4f

0 →	S	orbital
1 →	p	orbital
2 →	d	orbital
3 →	f	orbital

3. Magnetic quantum number (M_l) : The electrons present in particular sub-shell aquires certain specific orientation in space called orbital. These orientations are specified by quantum numbers called magnetic quantum number denoted by M_l

For every l, M_l varies from $-l$ to $+l$

Value of l	Value of M_l
$l = 0$	$M_l = 0$
$l = 1$	$M_l = -1, 0, +1$
$l = 2$	$M_l = -2, -1, 0, +1, +2$
$l = 3$	$M_l = -3, -2, -1, 0, +1, +2, +3$

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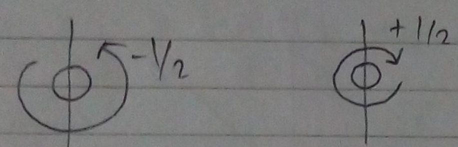
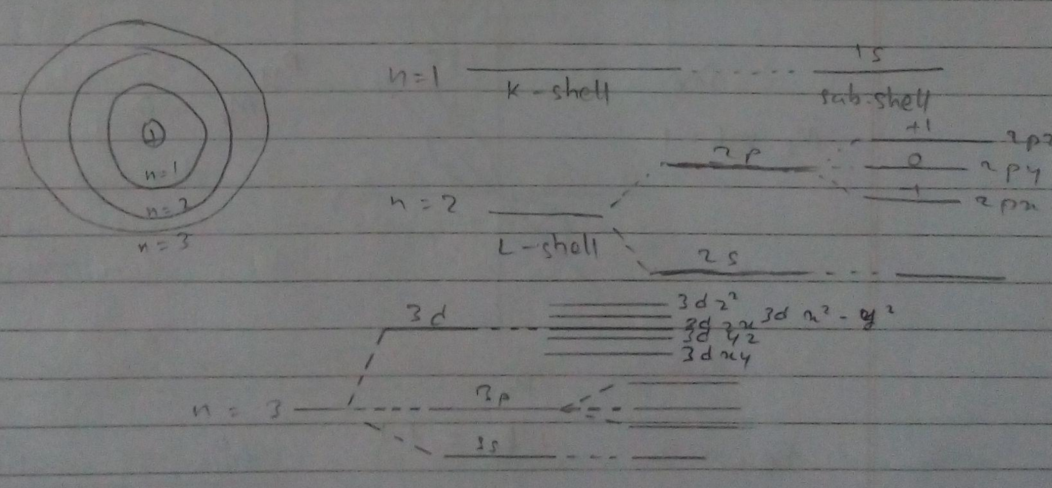
4. Spin quantum number (S/m_s): This number gives the information about the direction of spinning of electrons present in any orbital.

The electron in an orbital can spin either in clockwise direction or anti-clockwise direction. Hence for every given value of m, s can have two values, i.e., $+\frac{1}{2}$ or $-\frac{1}{2}$

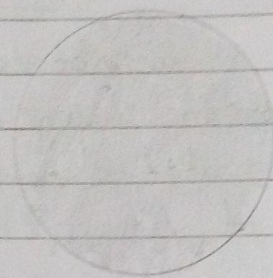


Summary

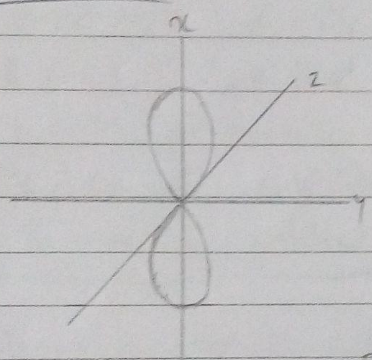


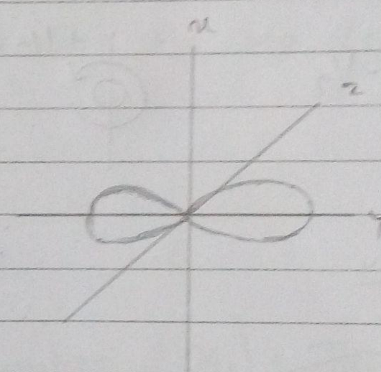
Shape of orbital.

1. S orbital →



2. P orbital -



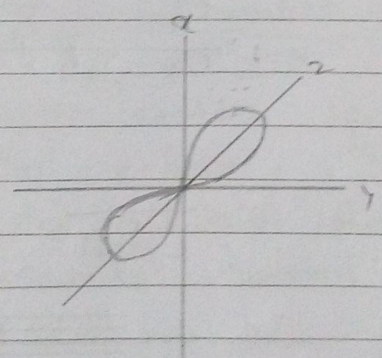


P_x

M_l ~~ml~~ $= -1$

P_y

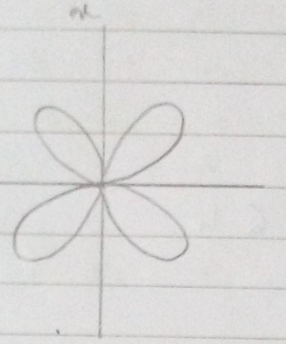
$M_l = 0$



P_z

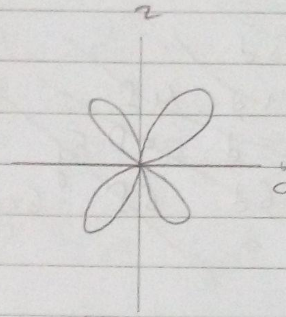
$M_l = +1$

3. d - orbital:



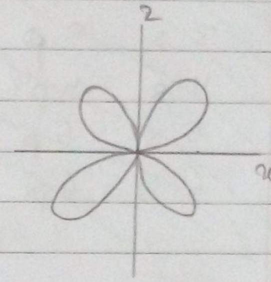
d xy

$m_l = -2$



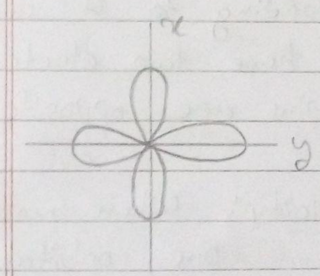
d yz

$m_l = -1$



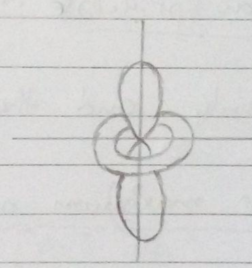
d xz

$m_l = 0$



d $x^2 - y^2$

$m_l = +1$



d z^2

$m_l = +2$

Filling of orbital in an atom.

1. Aufbau principle - In the ground state of an atom, the electrons are added progressively to the various orbital in increasing order of the energies

1 s
2 s 2 p
3 s 3 p 3 d
4 s 4 p 4 d 4 f
5 s 5 p 5 d 5 f 5 g
6 s 6 p 6 d 6 f 6 g 6 h

1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s

2. <u>Paulie's exclusion principle</u>: According to it an orbital can have two electrons at maximum only and their spins are opposite.

3. <u>Hund's rule for maximum multiplicity</u>: When more than one orbital of equal energies are available, the electrons will first occupy these orbitals singly with parallel spin. The pairing of electron will then take place.

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<u>Representation of electronic configuration of atom</u>

1 s
2 s 2 p
3 s 3 p 3 d
4 s 4 p 4 d 4 f

1 → H → $1s^1$

2 → He → $1s^2$

3 → Li → $1s^2\ 2s^1$

4. → Be → $1s^2\ 2s^2$

5. → B → $1s^2\ 2s^2\ 2p^1$

10 → Ne → $1s^2\ 2s^2\ 2p^6$

$p_x\ p_y\ p_z$

Ne → [↑↓] [↑↓] [↑↓|↑↓|↑↓]

1s 2s 2p

Na – $1s^2\ 2s^2\ 2p^6\ 3s^1$

Na – [Ne] $3s^1$

Ca – [Ar] $4s^2$

Ti

22 – Titanium – [Ar] $4s^2\ 4p^2$

Cl^- → 18 –

O^{2-} → 18 – ~~[Ne]~~ $2s^2\ 2p^6$

Fe^{2+} → 26 – [Ar] $3d^6\ 4s^2$

Q) Give the value of all 4 quantum number for 2p electrons in nitrogen.

Sol) N → 2p

$n = 2$

$p = 1$

$M_l = -1, 0, +1$

$s = +1/2, -1/2$

Q) Find all 4 ~~qu~~ quantum numbers for 3s.

$n = 3$

$l = \cancel{-3}, \cancel{+2}, 0$

$m_l = 0$

$s = +1/2, -1/2$

$\cancel{3p_z}$

Q) $n = 3, \ l = 1, \ m_l, \ s = -\frac{1}{2}$

$3p_2$

Q) $n = 4, \ l = 2, \ M_l = 2$

$4p_z$

$10 \rightarrow Ne \rightarrow 1s^2 \; 2s^2 \; 2p^6$

$11 \rightarrow Na \rightarrow 1s^2 \; 2p^2 \; 2p^6 \; 3s^1$

$\rightarrow [Ne] \; 3s^1$

$Al \rightarrow [Ne] \; 3s^2 \; 3p^1$

$Ar \rightarrow [Ne] \; 3s^2 \; 3p^6$

$K \rightarrow [Ar] \; 4s^1$

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