Lecture (1)

Energy Levels and Atomic Structure

The atom :

The atom is a basic unit of matter that consists of a dense central nucleus surrounded by a cloud of negatively charged electrons. The atomic nucleus contains a mix of positively charged protons and electrically neutral neutrons (except in the case of hydrogen-1, which is the only stable nuclide with no neutrons).

The atomic weight :

The mass of a given atom, measured on a scale in which the hydrogen atom has the weight of one. Because most of the mass in an atom is in the nucleus, and each proton and neutron has an atomic weight near one, i.e it is a ratio between the weight (mass) of atom in the matter to the weight of hydrogen atom.

$$W = m / w_H$$

Where

W: atomic weight
m: weight of atomic in the matter
w_H: weight of hydrogen atom
Note: atomic weight of H-atom = 1.008

The atomic number :

It is a number of protons in the nucleus of an atom. In electrically neutral atoms, this number is also equal to the number of electrons orbiting about the atom's nucleus. and is usually denoted by the letter *Z* and written as a subscript before an element's symbol, as in $_{92}U$.

Avogadro's number :

It is indicating the number of atoms or molecules in a mole of any substance , and its value is equal to 6.023 $\times 10^{23}$ mol^{-1} .

$$N_A = n / m$$

Where

N_A= Avogadro's number

n= No. of molecular

m= No. of moles

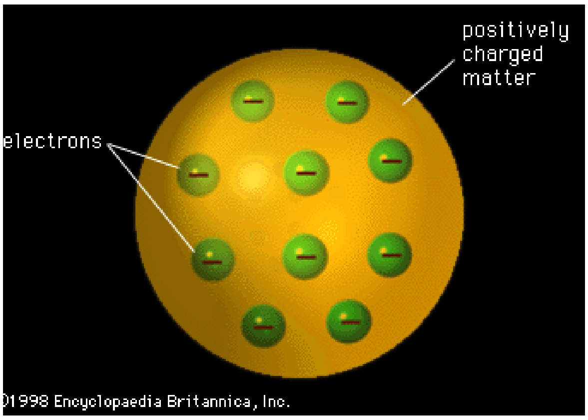
Models of atoms:

In order to investigate the different materials we must understand the structure of a single atom and its theory.

1-Thomson's Model

Thomson Model of the Atom

- J.J. Thomson discovered the electron and knew that electrons could be emitted from matter (1897).
- William Thomson proposed that atoms consist of small, negative electrons embedded in a massive, positive sphere.
- The electrons were like currants in a plum pudding.
- This is called the 'plum pudding' model of the atom.



And he calculated the charge of electrons $(1.6*10^{-19})$ coulomb and it's mass $=(9.1*10^{-31}$ kg).

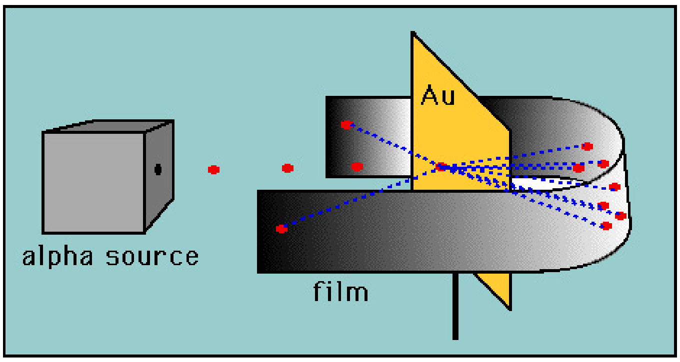
2-Rutherford's Model

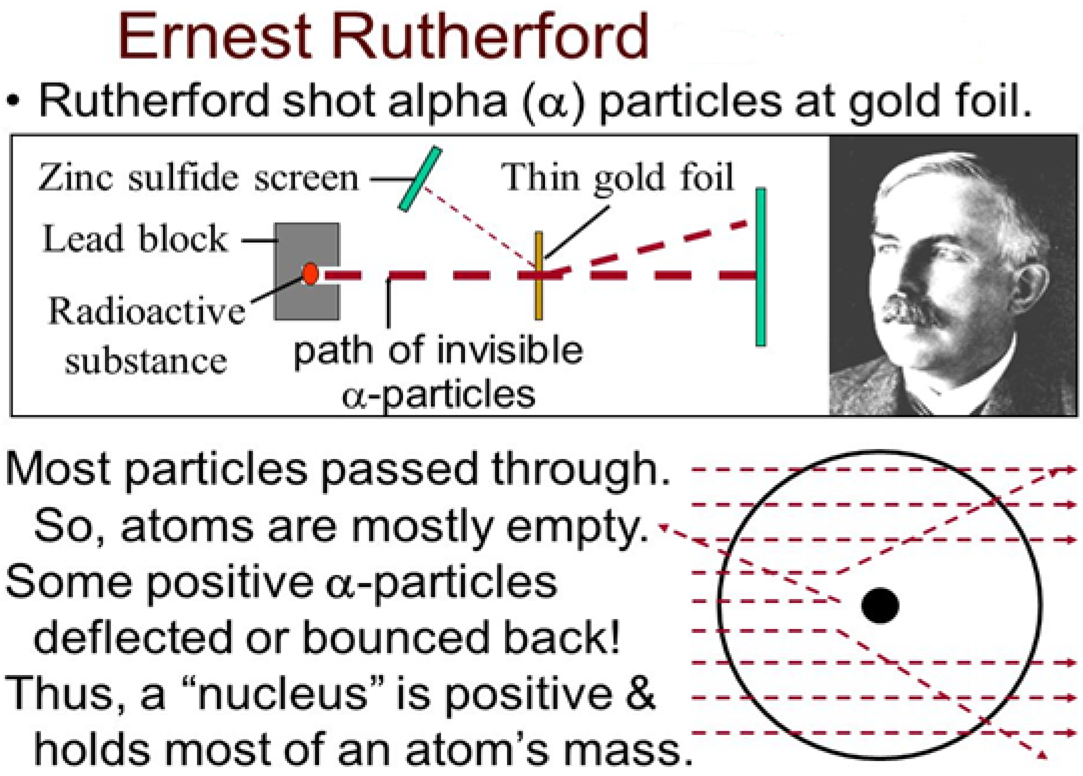
Rutherford overturned Thomson's model in 1911 with his well-known gold foil experiment in which he demonstrated that the atom has a tiny, heavy nucleus. Rutherford designed an experiment to use the alpha particles emitted by a radioactive element as probes to the unseen world of atomic structure. As expected, most alpha particles went right through the gold foil but to his amazement a few alpha particles rebounded almost directly backwards.

Rutherford's Gold Foil Experiment showed that:

1) Most of the mass of an atom (and all of its positive charge) is concentrated in a very small region in the center of an atom (the nucleus).

2) Most of the volume of an atom is empty space.





<u>Rutherford's postulates</u> :

1.Positive charged particle is present at the center of an atom and it is known as the nucleus which consists of the major mass of the atom.
2.The atoms are neutral due to the presence of equal charge of negatively charged electron and positive charged nucleus.
3.The electrons move around the nucleus as the planets move round the sun and the centrifugal force of nucleus is equal to the charge of the moving electrons.

<u>The strengths and weaknesses of Rutherford's atomic model:</u>

<u>strengths:</u> -electrons move fast through the atom. -electrons are trapped within the atom by a positively charged nucleus -electrons are negatively charged.

<u>weaknesses</u>: -failed to discover the nucleus contains positively charged particles called protons -failed to discover the nucleus also contains neutrons (a sub atomic neutral part).

When electrons rotate about nucleus , they have two types of forces:

<u>1-The attractive force F_e:</u>

It obtains between the electrons and the nucleus according Coulomb's law

$$F_e = e_1 e_2 / 4\pi\varepsilon_0 r^2 \qquad (1)$$

Where

$\mathbf{e_1 e_2}$:charges of nucleus and electron resp.

$\boldsymbol{\varepsilon_0}$: permittivity space = $8.85 * 10^{-12}$ F/m

r: radius (distance between two charges)

1-The centrifugal force F_c:

As result of the electrons circular orbital motion

$$\mathbf{F_c = m\upsilon^2/r} \qquad (2)$$

The two opposing forces just balance each of them and e_1=e_2 thus eqn. 1 = eqn.2

$$\mathbf{F = Ze^2/4\pi\varepsilon_0 r^2 = m\upsilon^2/r}$$

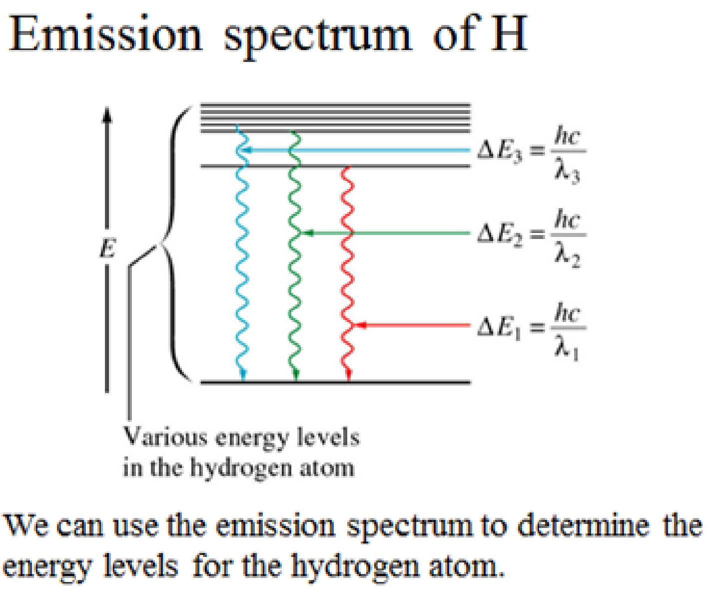
Then

$$\mathbf{\upsilon^2 = Ze^2/4\pi\varepsilon_0 m_e r} \qquad (3) \qquad \& \qquad \mathbf{r = e^2/4\pi\varepsilon_0\, \upsilon^2 m} \qquad (4)$$

the Maxwell's theory ,shows that electrons undergo a change in velocity will radius energy in the form of electromagnetic waves.

3-Bohr's Model:

The planetary model of Rutherford did not solve the problem completely, since electrons moving around the nucleus in an orbit were expected to lose energy, and thus eventually would spiral into the nucleus.
Bohr observed that when hydrogen is heated, only a few precise wavelengths of light are emitted. The spectrum produced when this light is passed through a prism is call the LINE or EMISSION SEPECTRUM.
When a Hydrogen atom is excited, the electron gains (absorbs) a certain quantity of energy and jumps from a lower a allowed energy level to a higher allowed energy level. The quantity of energy required for this promotion equals the difference in energy between the 2 energy levels.
When an electron drops back to a lower energy level l, the previously gained energy is given off in the form of radiation of a definite frequency. The frequency of the radiation depends on the amount of energy emitted (and can be calculated using the equation E = hv).
If the electron is already at the lowest energy level, no more energy can be emitted and therefore the atom does not collapse.
Since there are only certain allowed orbits or energy levels in the atom, the difference in energy between two allowed energy levels must also be a certain value. Thus, only certain energies can be absorbed or emitted as the electron changes orbits. This means that only certain frequencies of radiation can be absorbed or emitted as the electrons changes orbits since energy is directly proportional to frequency.



Bohr's postulates

1. Electrons revolve around the nucleus in circular path, which are known as "**ORBITS**" or "**ENERGY LEVEL**, this motion of an electron to be under the influence of the Coulomb attraction between the electron and the nucleus, obeying the laws of classical mechanics.
2. the Energy of an electron in one of its allowed orbits is fixed. As long as an electron remains in one of its allowed orbit, it cannot absorb or radiate energy .

3. Energy released or absorbed by an electron is equal to the difference of energy of two energy levels.
Let an electron jumps from a higher energy level E_2 to a lower energy level E_1.The energy is emitted in the form of light .Amount of energy released is given by:

$$\Delta E = E_2 - E_1 \qquad (5)$$

$$E_2 - E_1 = h\upsilon \qquad (6)$$

Where

h = Planck's consrant (6.6256 x 10^{-34} j.s)

υ= Frequency of radiant light

4. The angular momentum of an electron is given by:

$$L = n\hbar \qquad (7)$$
$$n = 1, 2, 3, \ldots$$

So

m v r = nh /2

Where n =1, 2, 3, ...

m = mass of electron

V = velocity of electron

r = radius of orbit

5.Instead of the infinity of orbits which would be possible in classical mechanics, it is only possible for an electron to move in an orbit for which its orbital angular momentum L is and integral multiple of $\hbar$.

6.Despite the fact that it is constantly accelerating, an electron moving in such an allowed orbit does not radiate electromagnetic energy. Thus, its total energy E.

For an electron moving in a stable circular orbit around a nucleus, Newton's second law reads

$$\frac{Ze^2}{r^2} = m\frac{v^2}{r}, \qquad (8)$$

where v is the electron speed, and r the radius of the orbit. Since the force is central, angular momentum should be conserved and is given by $L = |\mathbf{r} \times \mathbf{p}| = mvr$. Hence from the quantization condition of equation 7,

$$mvr = n\hbar. \qquad (9)$$

Equations 8 and 9 therefore give two equations in the two unknowns r and v. These are easily solved to yield Bohr radius

$$r = \frac{n^2\hbar^2}{mZe^2} = \frac{n^2}{Z}a_0 \qquad (10)$$

$$v = \frac{Ze^2}{n\hbar} = \frac{Z}{n}\alpha c, \qquad (11)$$

where

$$\alpha \equiv \frac{e^2}{\hbar c} \approx \frac{1}{137} \qquad (12)$$

is a dimensionless number known as the fine-structure constant for reasons to be discussed later. Hence αc is the speed of the electron in the Bohr model for the hydrogen atom (Z=1) in the ground state (n=1). Since this is the maximum speed for the electron in the hydrogen atom, and hence $v \ll c$ for all n, the use of the classical kinetic energy seems appropriate. From equation 8, one can then write the kinetic energy,

$$K = \frac{1}{2}mv^2 = \frac{Ze^2}{2r}, \qquad (13)$$

and hence the total energy,

$$E = K + V = \frac{Ze^2}{2r} - \frac{Ze^2}{r} = -\frac{Ze^2}{2r}. \qquad (14)$$

Having solved for r as equation 10, one can then write

$$E = -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{mc^2}{2}(Z\alpha)^2\frac{1}{n^2}. \tag{15}$$

Numerically, the energy levels for a hydrogenic atom are

$$E = -13.6\text{eV}\frac{Z^2}{n^2}. \tag{16}$$

i.e

$$E = -\frac{Zk_e e^2}{2r_n} = -\frac{Z^2(k_e e^2)^2 m_e}{2\hbar^2 n^2} \approx \frac{-13.6Z^2}{n^2}\text{eV} \tag{17}$$

Along with this excellent agreement with observation, the Bohr theory has an appealing aesthetic feature. One can write the angular momentum quantization condition as

$$L = pr = n\frac{h}{2\pi}, \tag{18}$$

where *p* is the linear momentum of the electron. Louis de Broglie's theory of matter waves predicts the relationship $p = h/\lambda$ between momentum and wavelength, so

$$2\pi r = n\lambda. \tag{19}$$

That is, the circumference of the circular Bohr orbit is an integral number of de Broglie wavelengths. This provided the Bohr theory with a solid physical connection to previously developed quantum mechanics.

Limitations of Bohr Model

1) electron couldn't circle around nucleus like a planet! Because they would lose energy (by emitting electromagnetic radiation) & spiral into nucleus.
2) The Bohr Model can only explain the line spectrum of hydrogen (an atom with only one electron) adequately
3) Scientists eventually concluded that Bohr's model did not fully describe the fine structure of an atom
4) It can't explain molecular bonds.

Rydberg formula for any hydrogen-like element

The formula above can be extended for use with any hydrogen-like chemical elements with

$$\frac{1}{\lambda_{\text{vac}}} = RZ^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \tag{20}$$

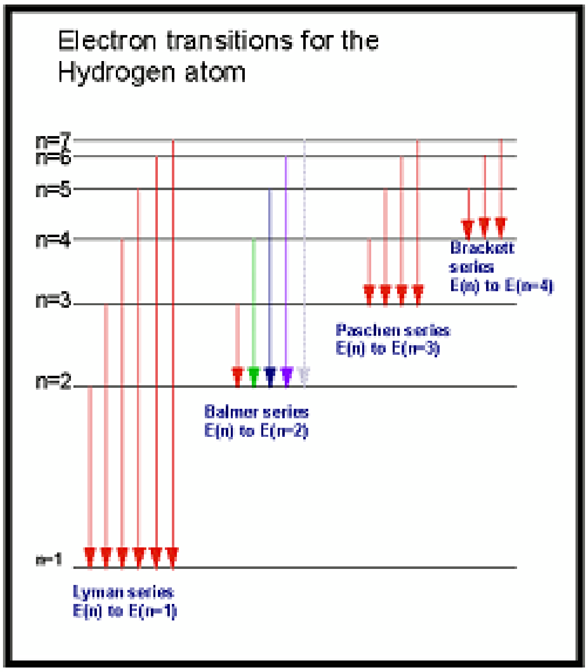
where

λ_{vac} is the wavelength of the light emitted in vacuum;

R is the Rydberg constant for this element;

Z is the atomic number, i.e. the number of protons in the atomic nucleus of this element;

n_1 and n_2 are integers such that



n_1	n_2	Name	Converge toward
1	$2 \rightarrow \infty$	Lyman series	91.13 nm (UV)
2	$3 \rightarrow \infty$	Balmer series	364.51 nm (Visible)
3	$4 \rightarrow \infty$	Paschen series	820.14 nm (IR)
4	$5 \rightarrow \infty$	Brackett series	1458.03 nm (Far IR)
5	$6 \rightarrow \infty$	Pfund series	2278.17 nm (Far IR)

$n_1 < n_2.$

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