Course Name: Chemistry
Course NO: CHE1203

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Atomic Structure

Dalton's Atomic Theory

Postulates

(a) All matters is composed of indivisible atoms. An atom is an extremely small particle of matter that retains its identity during chemical reaction.

(b) An element is a type of matter composed of only one kind of atom, each atom of a given kind having the same properties. e.g. mass

(c) A compound is a type of matter composed of atoms of two or more elements chemically combined in fixed proportions.

For example, water (H_2O) consists of hydrogen and oxygen atoms in the ratio of 2 to 1.

(d) A chemical reaction consists of the rearrangement of the atoms present in the reacting substances formed by the reaction.

Drawbacks of Dalton's Atomic Theory

➢The indivisibility of an atom was proved wrong: an atom can be further subdivided into protons, neutrons and electrons. However an atom is the smallest particle that takes part in chemical reactions.

➢According to Dalton, the atoms of same element are similar in all respects.

However, atoms of some elements vary in their masses and densities. These atoms of different masses are called isotopes. For example, chlorine has two isotopes with mass numbers 35 and 37.

➤Dalton also claimed that atoms of different elements are different in all respects. It is proven wrong in certain cases: Ar and Ca atoms each have an atomic mass of 40 amu. They are called isobars.

➤Atoms of different elements combine in simple whole number ratios to form compounds. This is not observed in complex organic compounds.

➤The theory fails to explain the existence of allotropes. For example charcoal, graphite, diamond.

Structure of Atom

Key Points

❑An atom is composed of two regions: the nucleus, which is in the center of the atom and contains protons and neutrons, and the outer region of the atom, which holds its electrons around the nucleus.

❑Protons and neutrons have approximately the same mass, about 1.67×10^{-24} g, which scientists define as one atomic mass unit (amu) or one Dalton.

❑Each electron has a negative charge (-) equal to the positive charge of a proton (+).

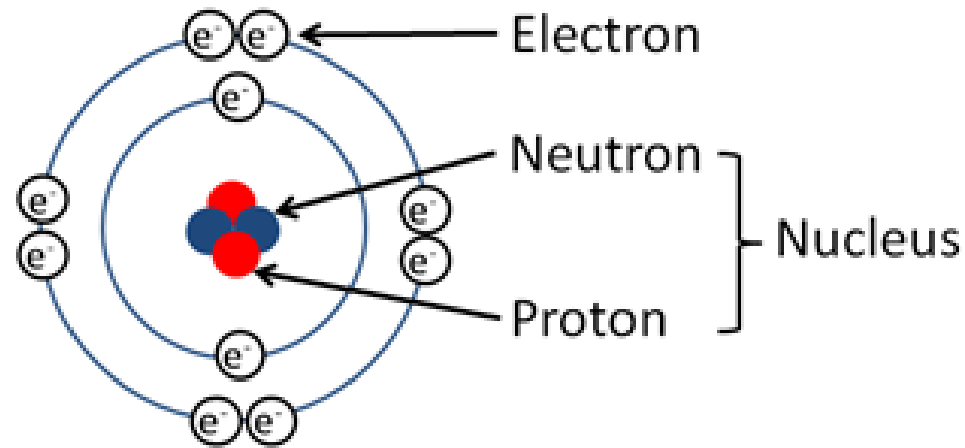❑Neutrons are uncharged particles found within the nucleus.

Fig. Schematic representation of Atom

Postulates of Rutherford Atomic Model

(a) An atom is composed of positively charged particles. Majority of the mass of an atom was concentrated in a very small region. This region of the atom was called as the nucleus of an atom

(b) The nucleus is surrounded by a number of electrons equal to the number of positive charge on it.

(c) The electrons are in constant motion round the nucleus like that of planets round the sun in such a way that the electrostatic force of attraction between the electrons and positive nucleus is counterbalanced by the centrifugal force.

Fundamental Particles of Atom

An atom is the smallest particle of an element having its own chemical identity and properties. But presently, we know that atoms can be subdivided into smaller sub-atomic particles known as fundamental particles. The fundamental particles of which atoms are composed are the proton, electron and neutron.

Atomic Number (Z)

The atomic number or proton number of a chemical element is the number of protons found in the nucleus of every atom of that element. The atomic number uniquely identifies a chemical element. It is identical to the charge number of the nucleus. Also identical to electron number of a neutral atom.

Atomic number (Z)= Proton No (p)=Electron No (e)

Mass Number (A)

The mass number (called atomic mass number) or nucleon number, is the total number of protons and neutrons in an atomic nucleus. The sum of the number of proton and neutron in a nucleus is A.
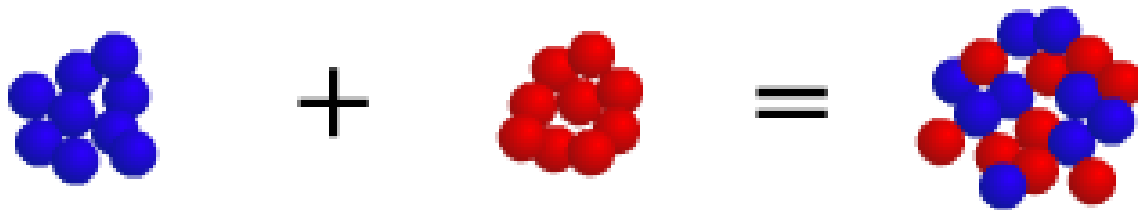
Mass number =
A = Z + N

Chemical symbol
for the element.

$$^{A}_{Z}X$$

Atomic number=
number of protons

N = neutron number

Z= Proton number (Z)

A= Mass number (Z+N)

Number of Neutrons + Number of Protons = Mass Number

Isotopes

The atoms of the same element having the same atomic number but different atomic mass number are called isotopes. For example, ^1_1H, ^2_1H, ^3_1H and $^{10}_6C$, $^{11}_6C$, $^{12}_6C$, $^{13}_6C$, $^{14}_6C$, $^{15}_6C$.
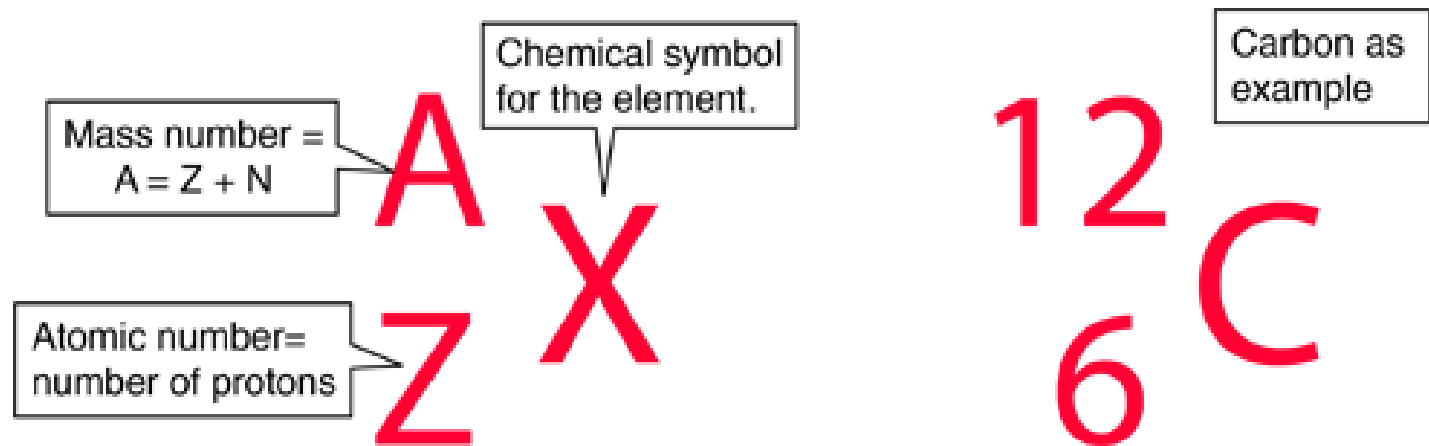
Isobars

Isobars are nuclides having the same mass number but different atomic number or proton number. For example, $^{12}_6C$ and $^{12}_5B$.

Isotones

Atoms of different elements having different mass number and same neutron number are called isotones. For example, $^{15}_7N$, $^{16}_8O$.

Nuclides

A nuclide is a particular nucleus characterized by a definite atomic number and mass number. For example, $^{23}_{11}\text{Na}$.

Chemical symbol for the element.

Mass number = $A = Z + N$

Atomic number = number of protons

$^{A}_{Z}X$

Carbon as example

$^{12}_{6}C$

Nucleons

The protons and neutrons in a particular nucleus together are called nucleons. For example, in $^{23}_{11}\text{Na}$, 11 protons and 12 neutrons are called nucleons.

The Wave Nature of Light

A wave is a continuously repeating change or oscillation in matter or in a physical field. Visible light, X-ray, and radio waves are all forms of electromagnetic radiation.

Amplitude

Crest

Fig. Water wave

Trough
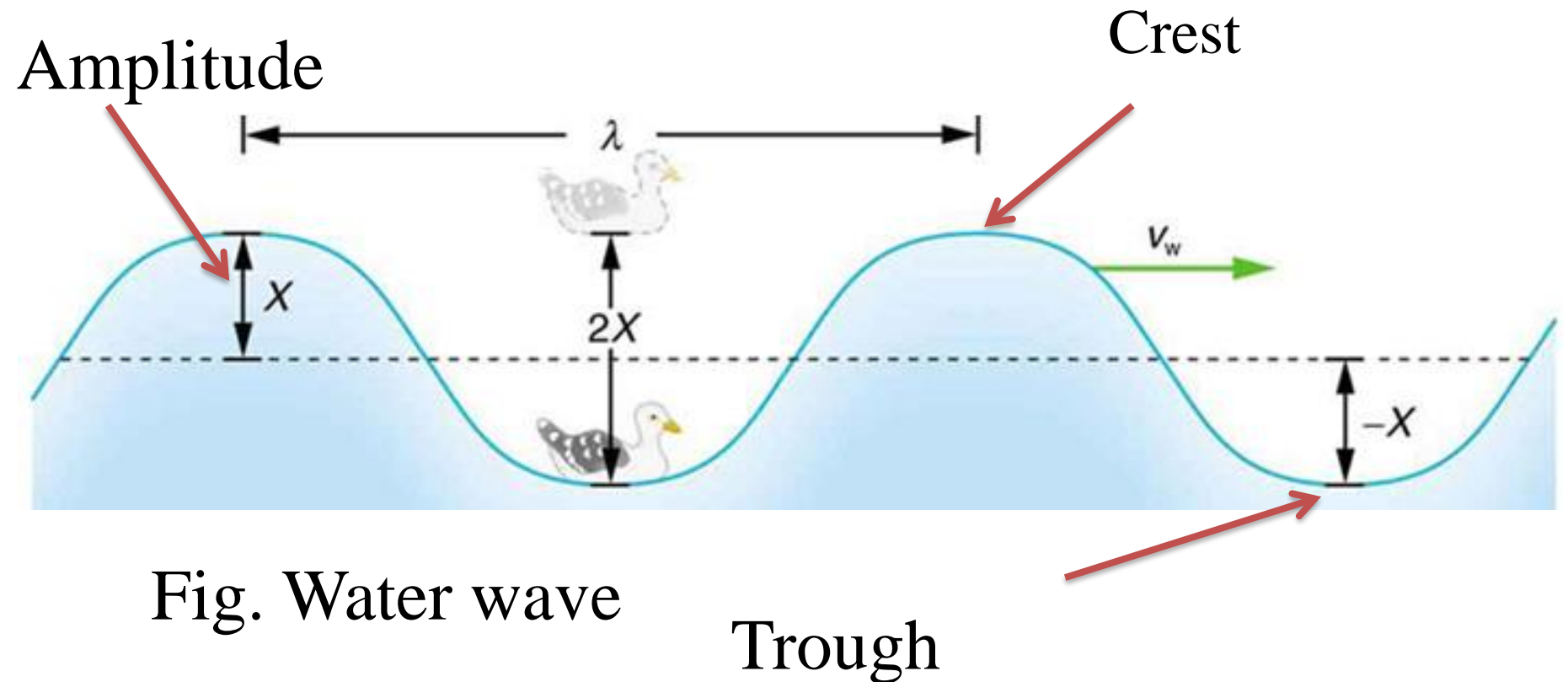
A wave is characterized by its wavelength (λ) and frequency (υ).

Wavelength (λ): The wavelength is the distance between any two adjacent identical points of a wave. It is denoted by λ. It's unit is nm, Å.

Frequency (υ): The frequency of a wave is the number of wavelengths of that wave that pass a fixed point in one unit of time (one second). It is denoted by υ. It's unit is Hertz (Hz), s^{-1}.

Relation between λ and υ

$$c = \upsilon\lambda \quad \text{or} \quad \lambda = c/\upsilon$$

Electromagnetic spectrum

The range of frequencies or wavelength of electro-magnetic radiation is called the electromagnetic spectrum.

Electromagnetic spectrum
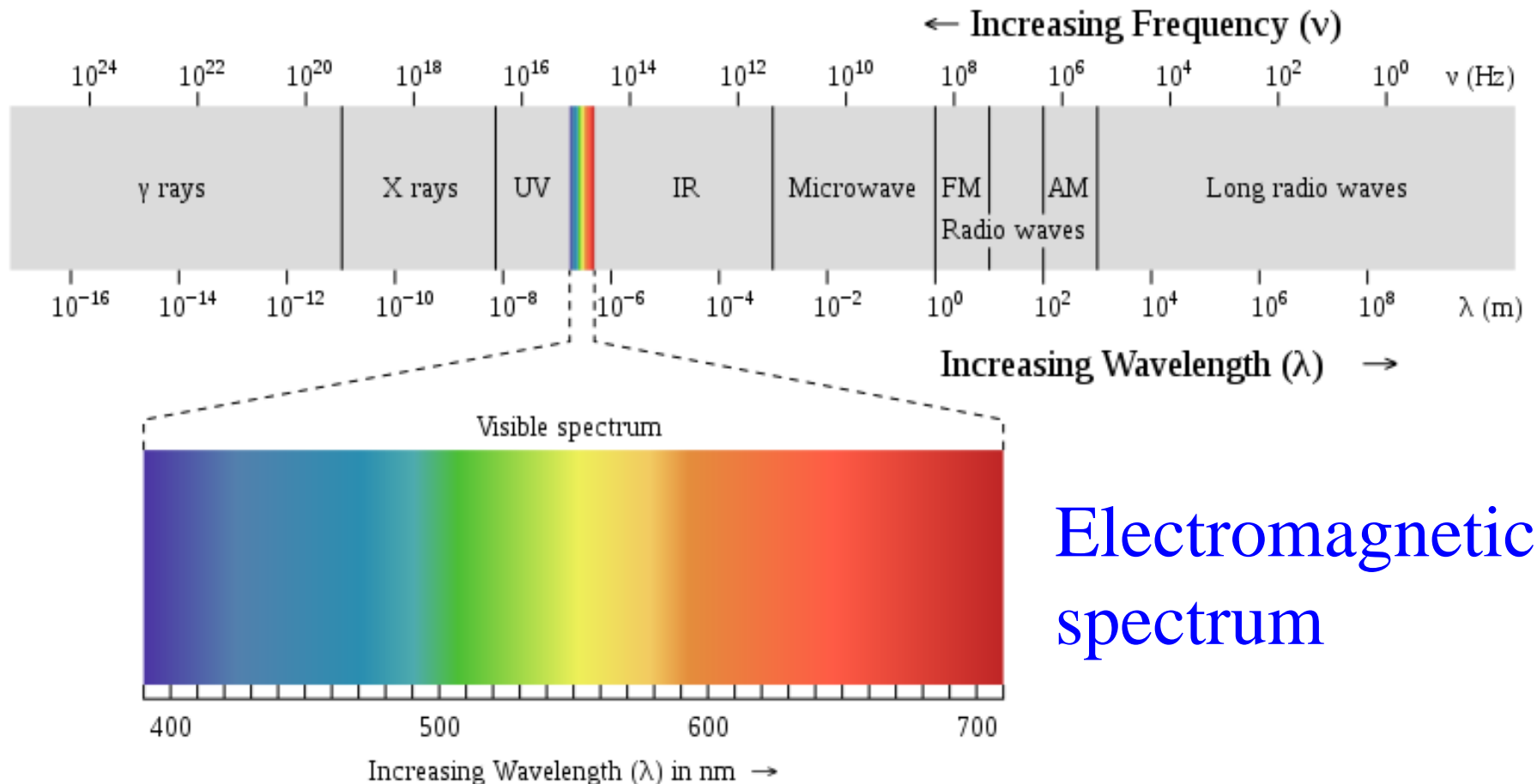
Planck's Quantization of Energy

According to Planck's theory of radiation, energy is radiated or absorbed by a body discontinuously in a definite fundamental unit or in an integral multiple of the fundamental unit. The unit of the energy was called by Planck 'a quanta'.

The magnitude of the unit of energy depends upon the frequency of radiation and thus a quantum of energy is directly proportional to the frequency of the radiation υ. In equation form this is expressed as,

$$\mathbf{E \propto \upsilon \; or \; E = h\upsilon}$$

This quantum of energy is known as photon resulting from one electronic transition. E is the unit of energy, and h, the Planck's constant. $h = 6.63 \times 10^{-34}$ J.s.

Photoelectric Effect

The photoelectric effect is the emission of electrons when electromagnetic radiation, such as light, hits a material. Electrons emitted in this manner are called photoelectrons. Electrons are ejected only when the frequency of light exceeds a certain threshold value. Increase the intensity of the incident radiation increase the number of electrons emitted per unit time.
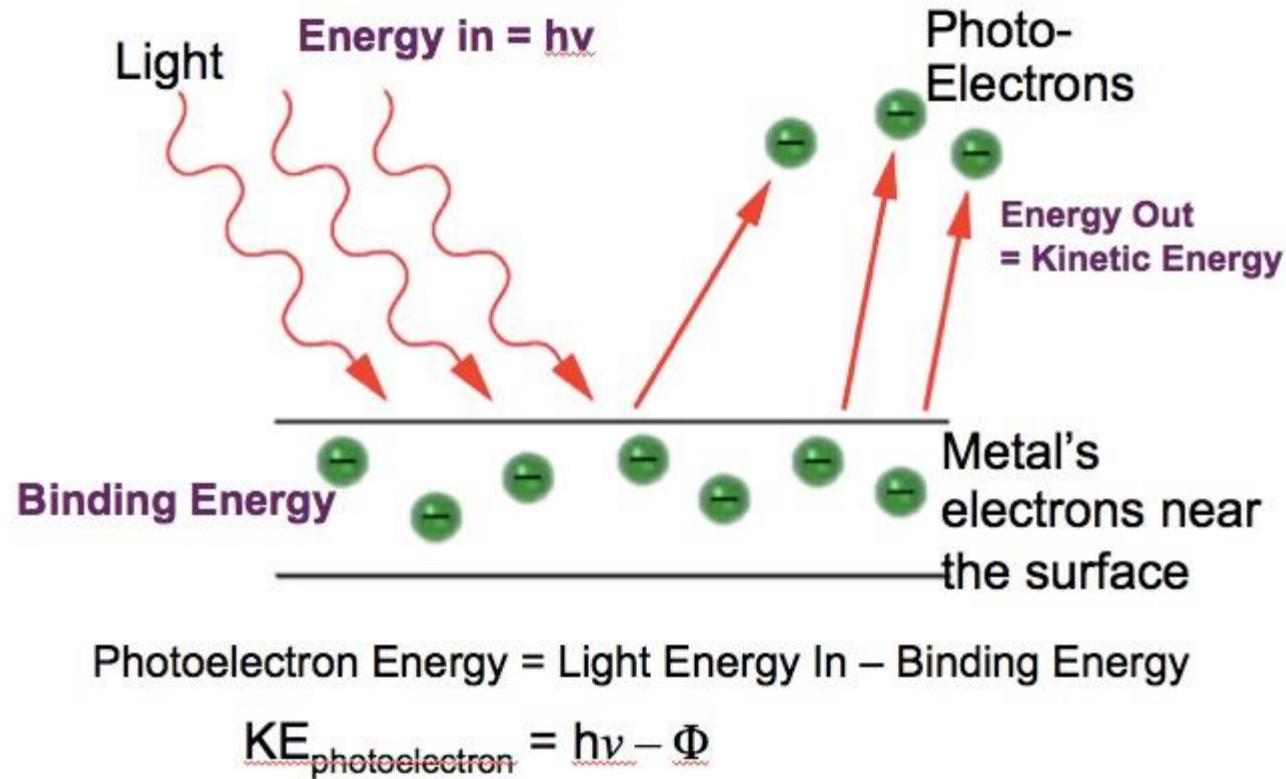
Fig. Schematic representation of Photoelectric effect

Atomic Line Spectra

When white is passed through a glass prism, diffraction occurs and the white light becomes separated into its component color known as spectrum.

A line spectrum: A spectrum showing only certain colors or specific wavelength of light is called line spectrum.

Fig. Atomic line spectrum

In the visible region, it consists of (hydrogen spectrum) only four lines (a red, a blue-green, a blue and violet), although others appear in the IR and UV regions.

In 1885 J.J. Balmer showed that the wavelengths λ in the visible spectrum of hydrogen could be reproduced by a simple formula:

$$\bar{\nu} = \frac{1}{\text{wave length}} = \frac{1}{\lambda} = 1.097 \times 10^7/\text{m} \ (1/2^2 - 1/n^2)$$

Here n is some whole number (integer) greater than 2. By substituting n=3, we find λ=6.56 x 10^{-7} m or 656 nm a wavelength corresponding to red light.
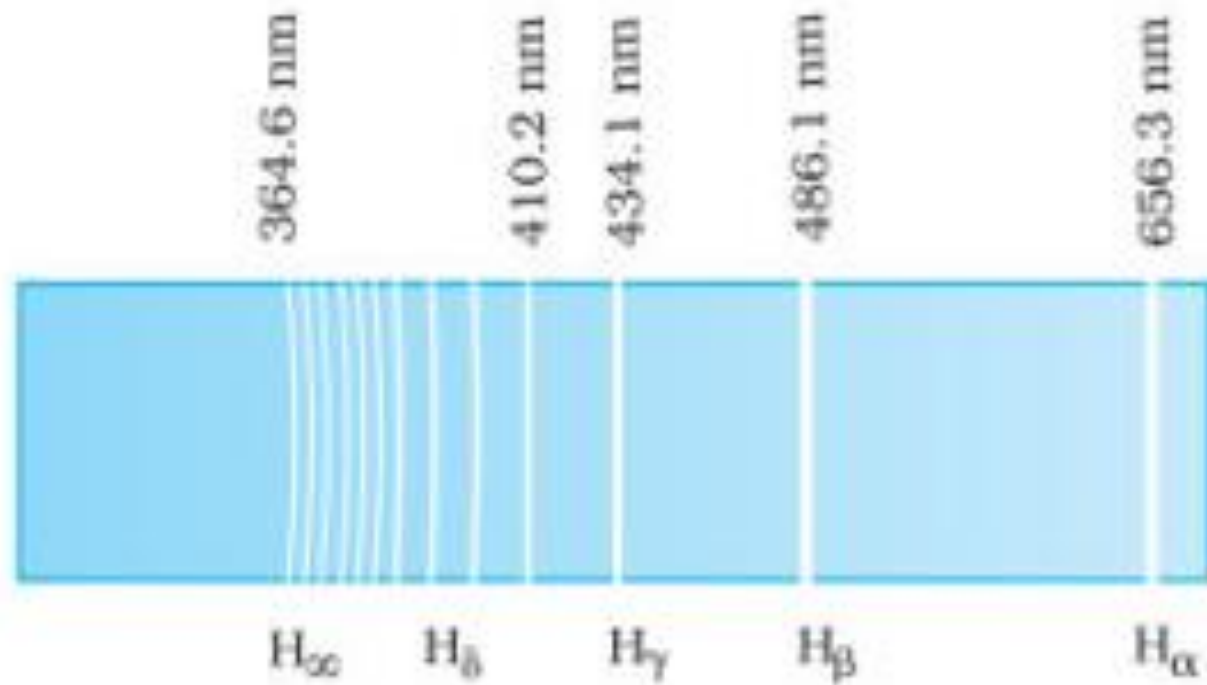
Fig. Balmer series of spectrum of hydrogen in the visible region.

Similarly, Lyman in 1906 studied the UV region of hydrogen spectrum and observed a number of lines, having the wavelengths in excellent agreement with the equation,

$$\frac{1}{\lambda} = \bar{\nu} = R_H \left(1/1^2 - 1/n^2 \right)$$

Where n is an integer having values 2, 3, 4, 5, etc. R_H is a constant known as Rydberg constant.

In 1908, Paschen discovered the series of lines in the infrared region of the hydrogen and a general equation was also derived.

$$\frac{1}{\lambda} = \bar{\nu} = R_H \left(1/3^2 - 1/n^2 \right)$$

Where n is an integer having values 4, 5, 6, etc.

In 1920, F.S. Bracket and 1924 A.H. Pfund discovered two series in the same region (IR) of hydrogen spectrum. This can be expressed by the equation,

$$\frac{1}{\lambda} = \bar{\nu} = R_H (1/n_1^2 - 1/n_2^2)$$

$$\text{Or} \quad \upsilon = R_H \, c \, (1/n_1^2 - 1/n_2^2)$$

Where c is the velocity of light, n_1 and n_2 are integers.

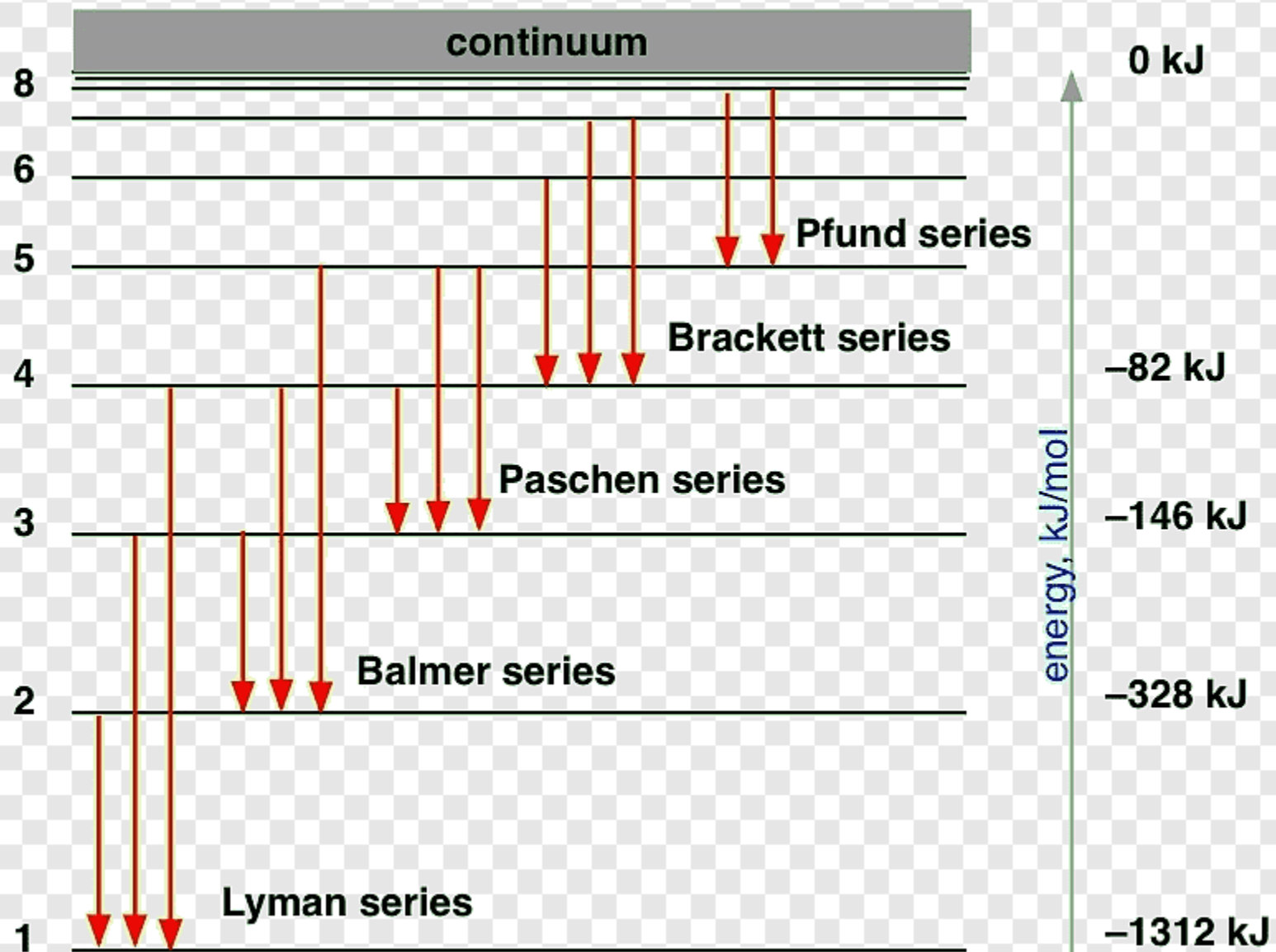| Series	n_2	n_1	Spectral region
Lyman	1	2, 3,4……..	UV
Balmer	2	3, 4,5…..	Visible
Paschen	3	4, 5, 6, ……	Near IR
Brackett	4	5, 6, 7, …..	Far IR
Pfund	5	6, 7, 8……..	Far IR
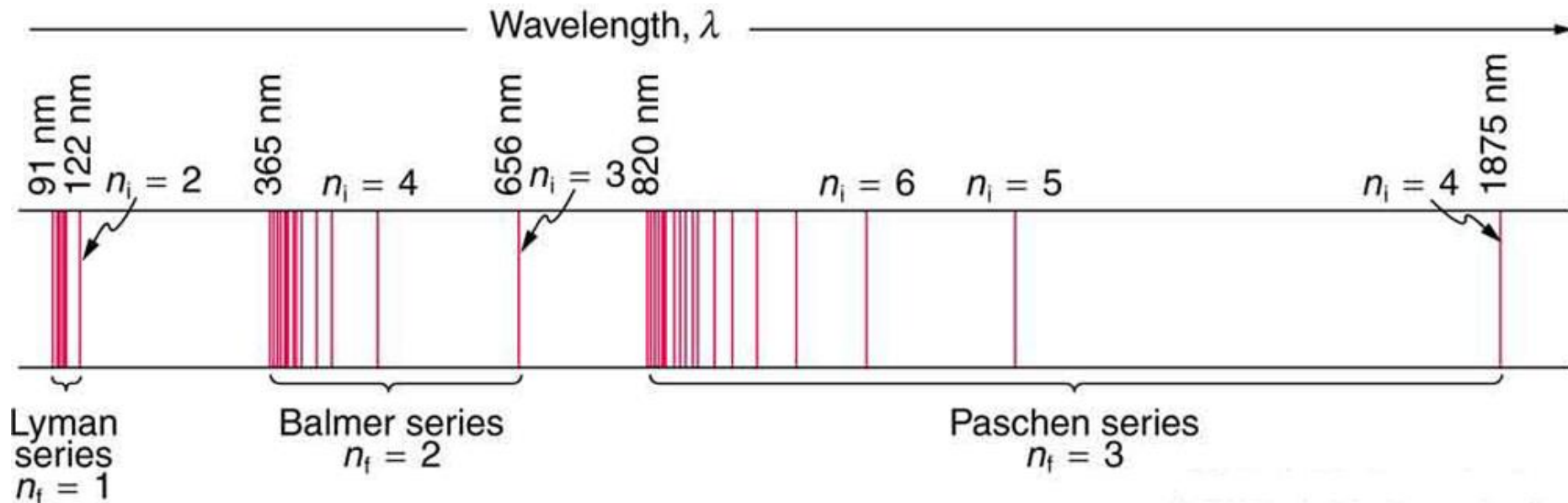
Fig. Different spectral series of hydrogen atom

Limitations of Rutherford Atom Model

Bohr pointed out that the Rutherford atom model is extremely unstable for the following reasons:

(a) Newton's laws of motion and gravitation can only be applied to neutral bodies such as planets and not to charged bodies such as tiny electrons moving round a positive nucleus. Since the electrons in an atom repel one another, whereas planets attract each other because of gravitational forces. Besides, there is electrostatic attraction in a nuclear atom model.

(b) According to Maxwell's theory, any charged body such as electrons rotating in an orbit must radiate energy continuously thereby loosing K.E.

Hence the electron must gradually spiral in towards the nucleus. The radius of the electron orbit will gradually decrease and it will ultimately fall into the nucleus, thus annihilating the atom model.

(c) Since the process of radiating energy would go on continuously, the atomic spectra should also be continuous and should not give sharp and well-defined lines.

Failure of Classical Physics

www.nuclear-power.net
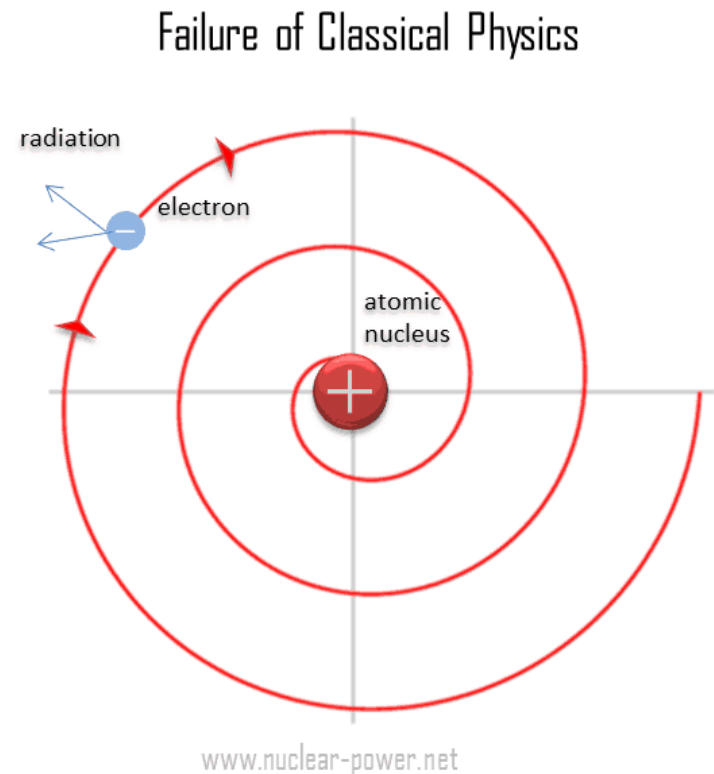
Bohr Atomic Model

Bohr Postulates

Bohr set down the following postulates to account for: (i) the stability of the hydrogen atom (that the atom exists and its electron does not continuously radiate energy and spiral into the radius) and (ii) the line spectrum of the atom.
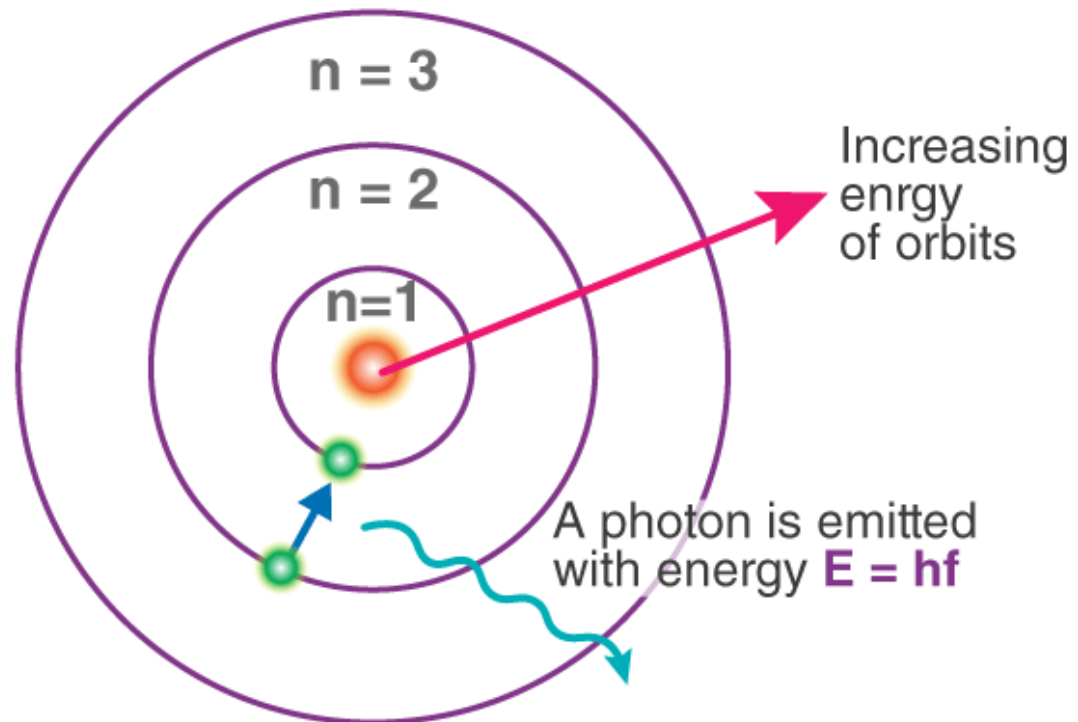
(a) **Postulate of Energy Levels**: An atom has a number of stable orbits in which an electron can revolve without the radiation of energy. These orbits are referred to as 'Energy levels'. Bohr devised a rule for the quantization that could be applied to the motion of an electron in an atom.

From this he derived the following formula for the energy levels of the electron in the hydrogen atom:

$E = -R_H/n^2$, n=1, 2, 3, ……$\propto$ (for H atom)

Where R_H is a constant with values of 2.179 x 10^{-18} J. Here n is called the principal quantum number.

Fig. Bohr
Model of
hydrogen atom

n = 3

n = 2

n=1

Increasing
enrgy
of orbits

A photon is emitted
with energy **E = hf**

(b) **Transition of electron between energy levels**: According to this postulate an electron can jump from one orbit to another. An atom radiates energy as light only when an electron passes from a higher energy level to lower energy level giving definite spectral lines in <mark>emission spectra</mark>. On the other hand, the jump of an electron from a lower energy level to that of higher energy level giving <mark>absorption spectra</mark> (dark line).

An electron in a higher energy level (initial energy level, Ei) undergoes a transition to a lower energy level (final energy level, Ef). In this process, the electron loses energy, which is emitted as a photon.

The final energy of the electron plus the energy of the photon equals the initial energy of the electron.

$E_f + h\upsilon = E_i$ or $E_i - E_f = h\upsilon$

Energy of emitted photon= $h\upsilon = E_i - E_f$.
In this postulate, Bohr used Einstein's photon concept to explain the line spectra of atoms. By substituting values of energy levels of the electrons in the H atom which had been derived, into the preceding equation, he has able to reproduce Balmer formula exactly. Moreover, he was able to predict all of the lines in the spectrum of the hydrogen atom, including those in the IR and UV regions.
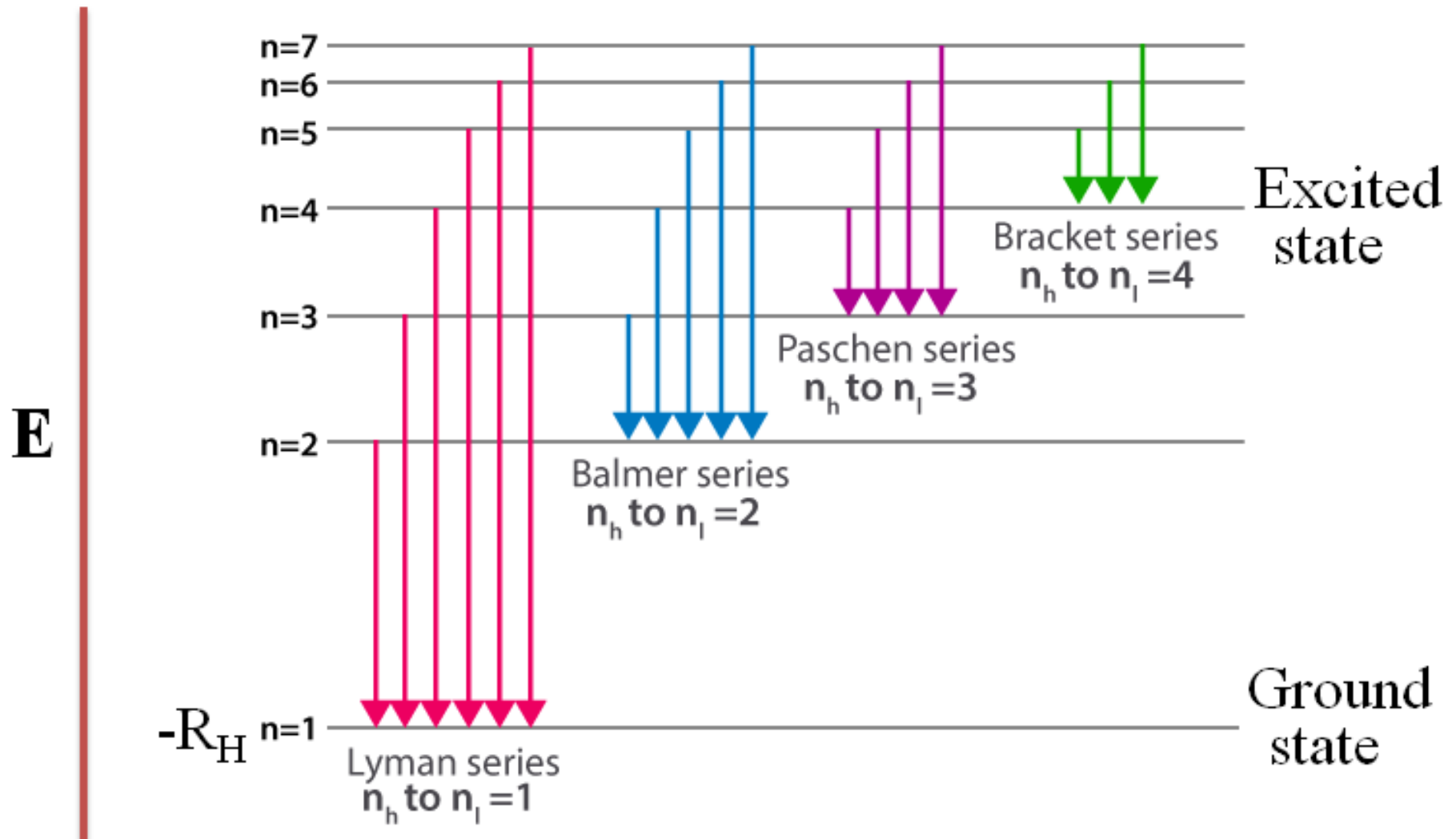
Fig. Energy level diagram showing energy levels of the hydrogen atom

Origin of Line Spectra

The emission line spectrum results from electrons dropping from higher energy level to lower energy levels. Each time an electron drops, a photon of light is released whose energy correspond to the difference in energy between the two levels.
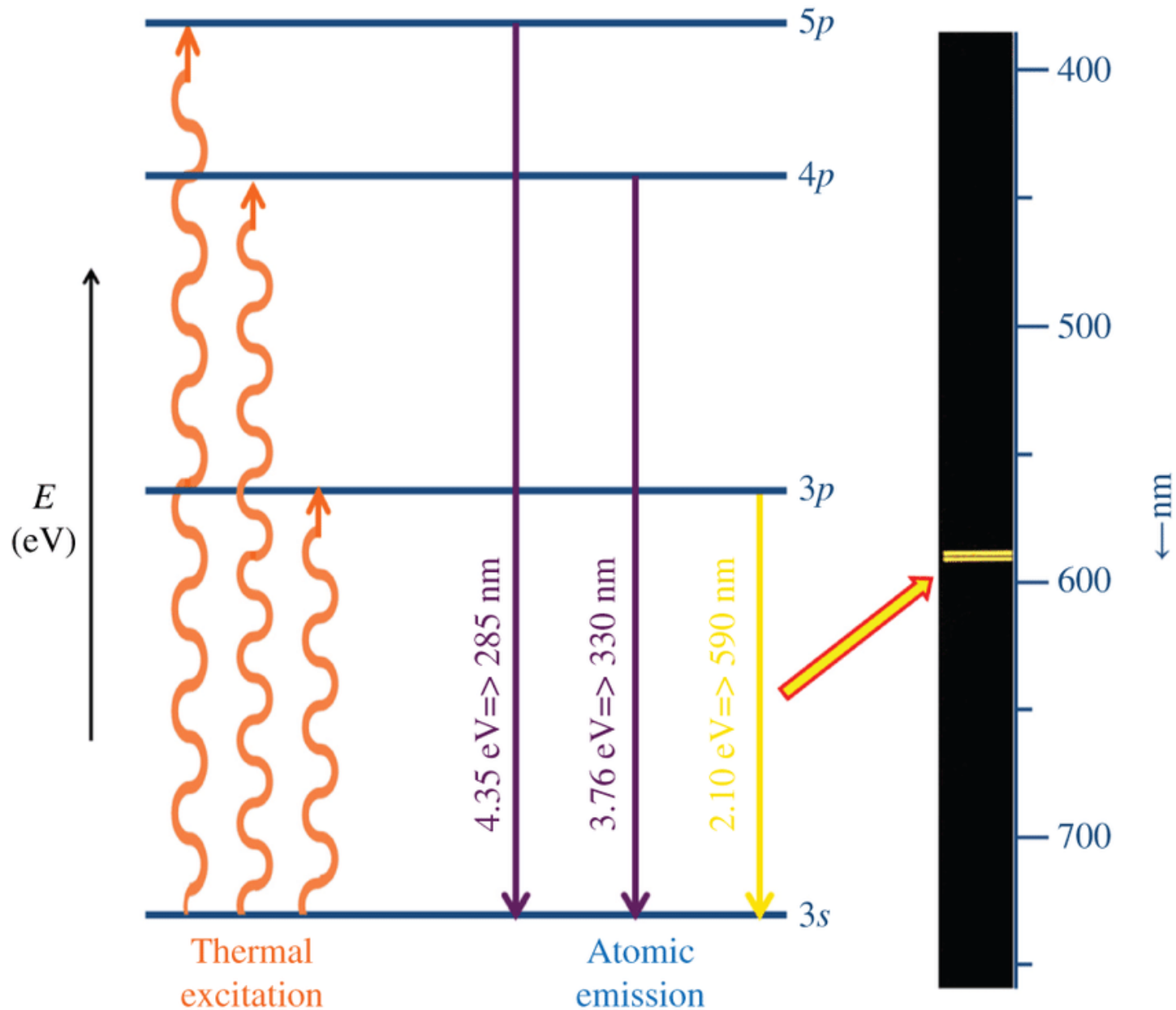
Violet: $n\lambda = d \sin\theta$, $\lambda = d \sin\theta/n = (1.0 \times 10^{-6}$ m$) \sin (24°) = 407$ nm

Blue: $n\lambda = d \sin\theta$, $\lambda = d \sin\theta/n = (1.0 \times 10^{-6}$ m$) \sin (25°) = 423$ nm

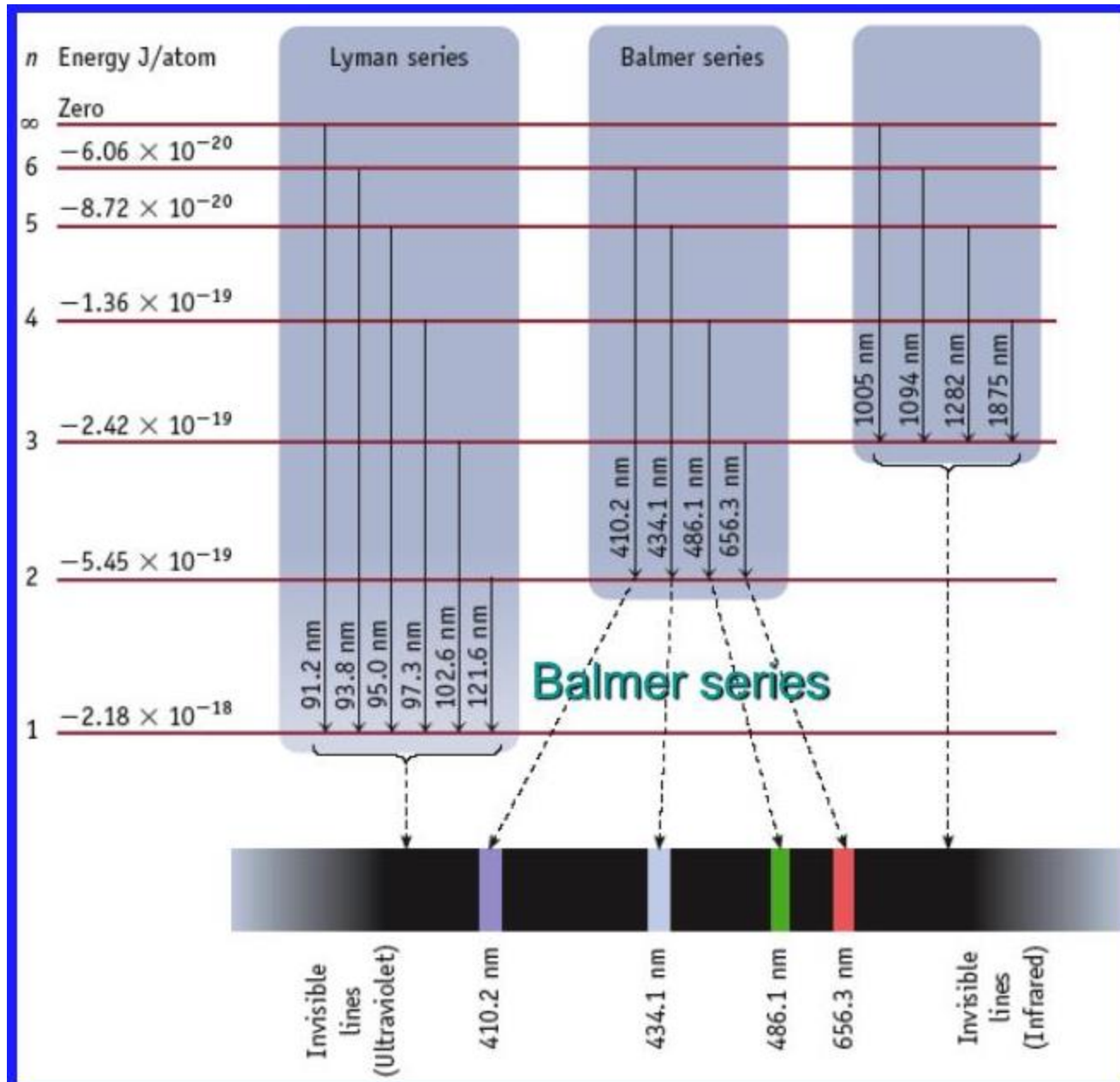**Green**: $n\lambda = d \sin\theta$, $\lambda = d \sin\theta/n = (1.0 \times 10^{-6}$ m$) \sin (29°) = 485$ nm

Red: $n\lambda = d \sin\theta$, $\lambda = d \sin\theta/n = (1.0 \times 10^{-6}$ m$) \sin (42°) = 407$ nm

Origin of Line spectra

Different regions of the line spectrum

According to Bohr theory

Lyman series →
Any energy level to lowest level (n=1)

Balmer series →
Any energy level to n=2 level

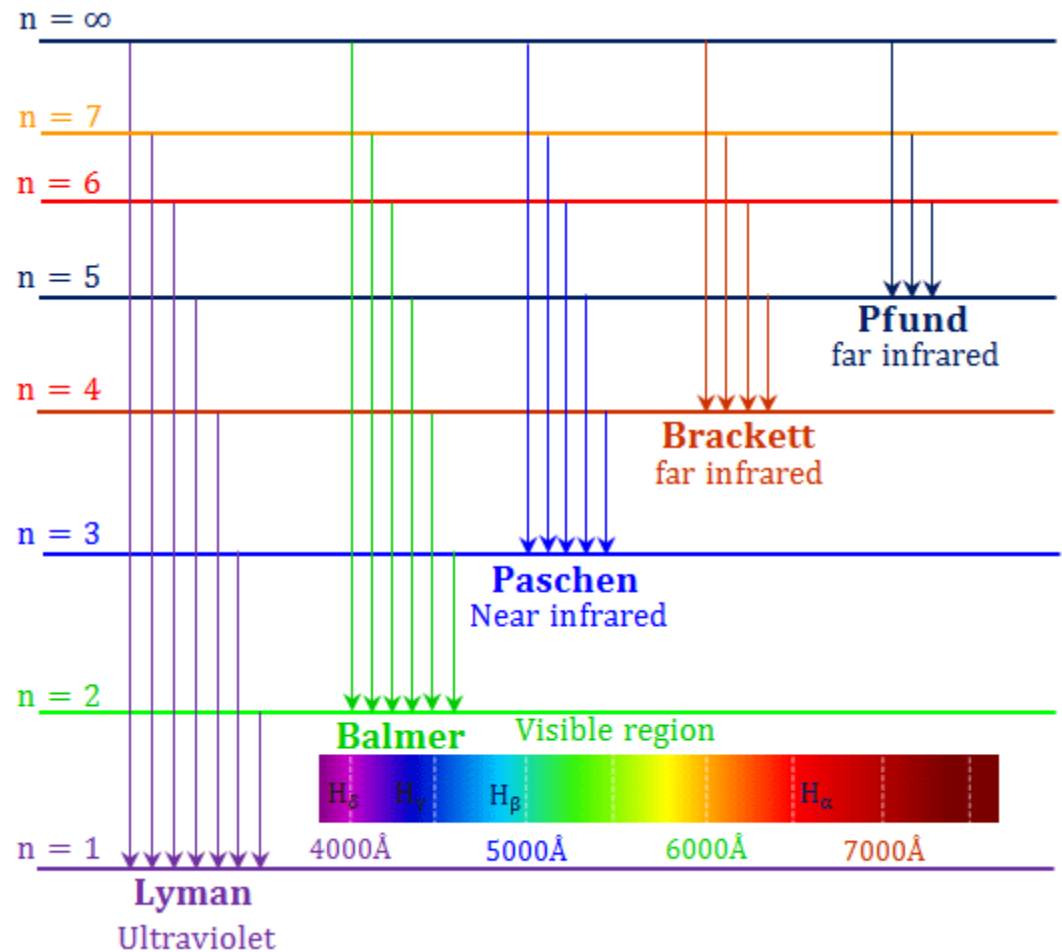Paschen series →
Any energy level to n-3 level

Fig. Origin of emission spectra of hydrogen atom

Limitation of Bohr Theory

(a) Bohr theory was successful in explaining the spectrum of hydrogen but failed to predict the energy states of more complicated atoms for more than one electron.

(b) Periodic motion around a central body usually follows an elliptical path rather than a circular path which has been assumed in the case of Bohr theory. If electrons follow elliptical path, the velocity along the path does not remain constant. Following Fig. indicates the precession of electron orbit due to changes in the velocity of the electron in elliptical orbit with the nucleus at one of the foci.

(c) Multiple lines in the atomic spectra has been found but the multiple lines has not been explained by Bohr theory.

(d) It does not explain the Zeeman Effect, when the spectral line is split into several components in the presence of a magnetic field.

(e) It is in violation of the Heisenberg Uncertainty Principle.
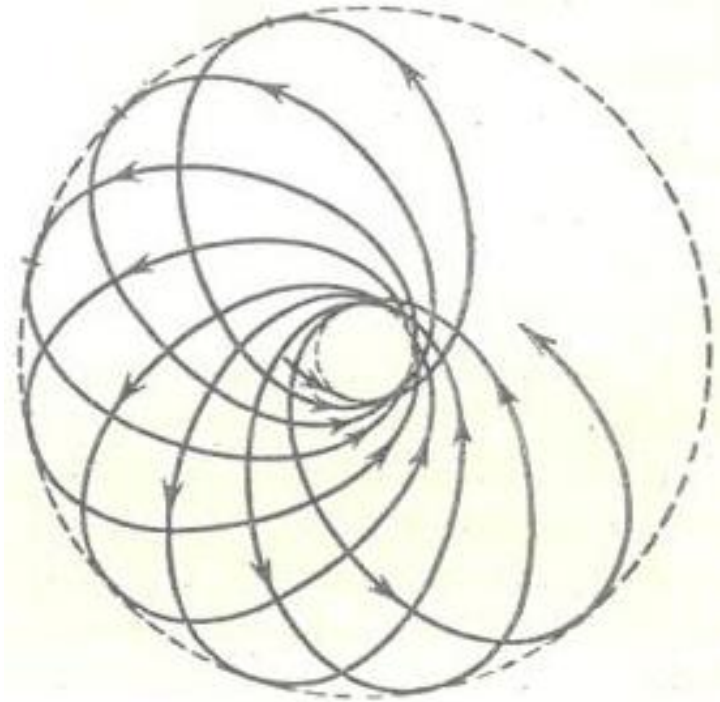

Fig. Precession of the electron orbit due to changes in the velocity of the electron.

The Bohr Model considers electrons to have both a known radius and orbit, which is impossible according to Heisenberg.

Problem: What is the wavelength of light emitted when the electron in a hydrogen atom undergoes a transition from energy level n=4 to level n=2?

Solution:

From the formula for the energy level,

$E_i = -R_H/4^2 = -R_H/16$ and $E_f = -R_H/2^2 = -R_H/4$

Now, $-R_H/16 - (-R_H/4) = -4R_H + 16R_H/64 = -R_H + 4R_H/16$

$= 3R_H/16 = h\upsilon$

The frequency of light emitted is

$\upsilon = 3R_H/16h = 3/16 \times 2.179 \times 10^{-18}$ J$/6.63 \times 10^{-34}$ J.s.

$= 6.17 \times 10^{14}$ /s

Since, $\lambda = c/\upsilon = 3.0 \times 10^8$ m/s$/6.17 \times 10^{14}$ /s

$= 4.86 \times 10^{-7}$ m $= 486$ nm

The color of the light is blue-green.

Problem: The red spectral line of lithium occurs at 671 nm (6.71×10^{-7}m). Calculate the energy of one photon of this light.

Solution:

The frequency of this light is

$\upsilon = c/\lambda = 3.0 \times 10^8$ m/s $/6.71 \times 10^{-7}$m $= 4.47 \times 10^{14}$/s

The energy of one photon is
$E = h\upsilon = 6.63 \times 10^{-34}$ J.s. $\times 4.47 \times 10^{14}/s = 2.96 \times 10^{-19}$ J

Wave Nature of Electrons

Einstein first proposed that light consists of discrete units of energy known as photons, which was later confirmed by the photoelectric effect experiment. This dual nature of light became known as the wave-particle duality. Louis de Broglie extended the wave-particle duality to electron; he argued that electrons not only act as particles but can also act as waves. The Daviscon-Geimer experiment later confirmed the wave nature of electrons.

Electrons were accelerated at a metal surface and scattered to form a diffraction pattern that can only be explained using wave particles.

De Broglie Wave Equation

According to theory of radiation, E, is the energy of radiation, is related to υ by the expression

$$E = h\upsilon \qquad \text{(i)}$$

Again, according to Einstein, the light has not only wave properties, but also particle properties.

$$E = mc^2 \qquad \text{(ii)}$$

From Eqns (i) and (ii) we get

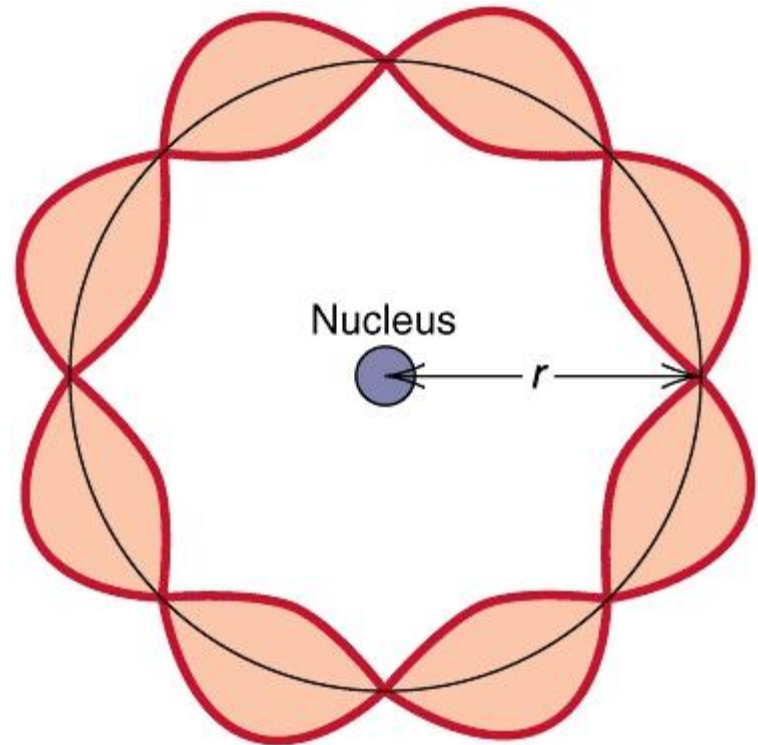$$mc^2 = h\upsilon \quad \text{or } mc = h\upsilon/c = h/\lambda \quad [\text{since, } \upsilon = c/\lambda]$$

Hence, $\lambda = h/mc$ (iii)

Applying Eq^n (iii) on electron moving with velocity v and associated with wavelength λ, de Broglie obtained.

$$\lambda = h/mv \qquad (iv)$$

This is de Broglie relation

Fig. Electron cloud of a stationary wave

Nucleus

r

Heisenberg Uncertainty Principle

According to this principle, it is impossible to determine accurately both the exact position and exact energy of an electron simultaneously. Therefore, more accurately we measure the energy of a moving electron, the less accurately we can determine its position and vice versa.

Mathematically

It is a relation that states that the product of the uncertainty in position and the uncertainty in momentum of a particle can be no smaller than Planck's constant divided by 4π. Thus letting Δx be the uncertainty in the x coordinate the particle

position and letting Δp_x, be the uncertainty in the momentum in the x direction, we have

$$(\Delta x)(\Delta p_x) \geq h/4\pi$$

There are similar relation in the y and z directions.

The Schrödinger Wave Equation

The Schrödinger equation is a linear partial differential equation that describes the wave function or state function of a quantum-mechanical system. The Schrödinger equation can be written as

Second derivative with respect to Z

Schrodinger wave Function

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

Position

Energy

Potential Energy

Where E is total energy, v is potential energy, m is mass of electron, h is Planck's constant, and ψ is wave function.

Significance of ψ function

ψ function has no physical significance but its square ψ^2 gives the probability of finding the particle within a region of space. The wave function and it square, ψ^2 have values for all location about a nucleus. The wave function describe the position of the particle w. r. t. time.

Figure shows values of ψ^2 for the electron in the lowest energy level of the hydrogen atom along a line starting from the nucleus.
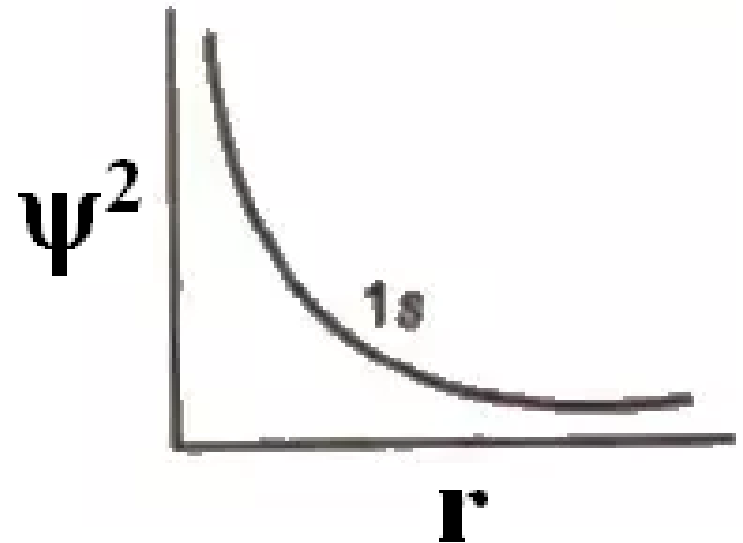
ψ^2 is larger near the nucleus (r=0),indicating that the electron is most likely to be found in this region. The values of ψ^2 decreases rapidly as the distance from the nucleus increases, but ψ^2 never goes to exactly zero, although the probability becomes extremely small at large distance from the nucleus.

Quantum Number

The set of numbers used to describe the position and energy of the electron in an atom are called quantum numbers. There are four quantum numbers, namely, principal quantum number (n), azimuthal/subsidiary quantum number (l), magnetic quantum number (m) and spin quantum number (s).

According to quantum mechanics, each electron in an atom is described by four different quantum numbers, three of which (n, l and m) specify the wave function that gives the probability of finding electron at various points in space. A fourth q. n. (s) refers to a magnetic property of electron called spin q. n.

(i) **Principal Quantum Number (n):** This q. no. is the one on which the energy of an electron in an atom principally depends. It can have any positive values: 1, 2, 3, and so on. The energy of an electron in an atom depends principally on n.

Significances

(a) The values of n represents the shell or energy levels in which the electrons revolves round the nucleus. Shells are sometimes designated by the following letters:

Letter K L M N…………

n   1 2 3 4 …………

(b) n also determines the location of the electron in a shell, i.e. n determines the distance of the electron from the nucleus.

(c) n also determines the energy of the electron in a given orbit.

(d) n determines the max. no. of electrons that a shell can hold. A shell with principal q. no. n can have $2n^2$ electrons.

(ii) Azimuthal/subsidiary q. no. (l)

This q. no. distinguishes orbitals of given n having different shapes; it can have any integer value from 0 to n-1.

Within each shell of q. no. n, there are n different kinds of orbitals, each with a distinctive shape denoted by l q. no.

Significances
(a) Orbitals of the same n but different l are said to belong to different sub-shells of a given shell. The different sub-shells are usually denoted by as follows:
Letter   s p d f g...........
l values   0 1 2 3 4...........
s=sharp, p=principal, d=diffuse and f=fundamental
(b) Values of l define the shape of the sub-shell (electron cloud) occupied by the electron

i.e. whether the sub-shell is spherical, dumpbell or with some other complicated shape.

(c) l values enable us to calculate the total no. of sub-shells which a main shell (K, L, M) has. The total number of sub-shells in a main shell with principal q. no. n is equal to the total number of l values for the given value of n.

(d) l values also enable us to calculate the total number of electrons in a given sub-shell. Total number of electrons in a given sub-shell with a given l values is equal to $2(2l+1)$. Thus, s, p, d, f sub-shells have 2, 6, 10 and 14 electrons.

(iii) Magnetic q. no. (m)

This q. no. distinguishes orbitals of given n and l that is given energy and shape but having a different orientations in space; the allowed values are the integers from $-l$ to $+l$ including zero.

Significances

(a) All the orbitals of the same sub-shell differ in the direction of their space orientation. For example $2p_x$, $2p_y$ and $2p_z$ orbitals which belong to the same sub-shell $2p$ (n=2, l=1) have different space orientations.

(b) The total no. of orbitals in a given sub-shell (for a given value of l) is equal to the total no. of m values.

(c) Total no. of orbitals in a main shell is equal to the total no. of m values for a given value of l. In terms of n, no. of orbitals in the nth shell is equal to n^2.

(iv) Spin q. no. (s)

The spin quantum number (s) describes the angular momentum of an electron. An electron spins around an axis and has both angular momentum and orbital angular momentum. Because angular momentum is a vector, the Spin Quantum Number (s) has both a magnitude (1/2) and direction (+ or -). The electron spins about its own axis either in a clockwise or in an anticlockwise.

Significances

This q. no. is needed to describe a property of the electron itself, which is not the property of the orbital.

Name	Symbol	Allowed Values	Property
Principal	n	positive integers 1,2,3…	Orbital size and energy level
Secondary (Angular momentum)	l	Integers from 0 to (n-1)	Orbital shape (sublevels/subshells)
Magnetic	m	Integers $-l$ to $+l$	Orbital orientation
Spin	s	$+\frac{1}{2}$ or $-\frac{1}{2}$	Electron spin Direction

Principal quantum number	Azimuthal quantum number	Magnetic quantum number	Spin quantum number	Total number of electrons in s, p, d orbital
$n = 1$ (K shell)	$l = 0$ (1S)	$l = 0$ (1S)	$+\frac{1}{2}, -\frac{1}{2}$	2
$n = 2$ (L shell)	$l = 0$ (2S)	$m = 0$ (2S)	$+\frac{1}{2}, -\frac{1}{2}$	2
	$l = 1$ (2P)	$m = 0$ ($2P_x$) $m = +1$ ($2P_y$) $m = -1$ ($2P_z$)	$+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$	$\left. \begin{array}{c} 2 \\ 2 \\ 2 \end{array} \right\} 6$
$n = 3$ (M shell)	$l = 0$ (3S)	$l = 0$ (3S)	$+\frac{1}{2}, -\frac{1}{2}$	2
	$l = 1$ (3P)	$m = 0$ ($3P_x$) $m = +1$ ($3P_y$) $m = -1$ ($3P_z$)	$+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$	$\left. \begin{array}{c} 2 \\ 2 \\ 2 \end{array} \right\} 6$
	$l = 2$ (3d)	$m = 0$ ($3d_{xy}$) $m = +1$ ($3d_{yz}$) $m = -1$ ($3d_{zx}$) $m = +2$ ($3d_{x^2-y^2}$) $m = -2$ ($3d_{z^2}$)	$+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$ $+\frac{1}{2}, -\frac{1}{2}$	$\left. \begin{array}{c} 2 \\ 2 \\ 2 \\ 2 \\ 2 \end{array} \right\} 10$

n=1, 2, 3…….
l= 0, (n-1)
m= -l to +l including 0

If n=2
Then
l= 0, (n-1)=(2-1)=1 i.e.0, 1
Then
m= 0, -1, +1

Pauli Exclusion Principle

No two electrons in the same atom can have the same values for the four quantum numbers.

Or No two electrons in the same atom can have identical sets of four quantum numbers.

Thus two electrons of the same atom can have the same values for three of their q. nos., but the fourth q. no. must be different for the two electrons. Thus two electrons may have orbitals of the same size, shape and orientation in space provided they have opposed spins.

Distribution of Electrons in the Atoms of Elements

Principal Q. No.	Max. No. of Electrons	No. of Electrons distributed in orbitals
1	2	$1s^2$
2	8	$2s^2 2p^6$
3	18	$3s^2 3p^6 3d^{10}$
4	32	$4s^2 4p^6 4d^{10} 4f^{14}$
5	32	$5s^2 5p^6 5d^{10} 5f^{14}$

The max. no. of electrons which the different types of atomic orbitals can accommodate are: s→2, p→6, d→10 and f→14

Aufbau Principle (Building up Principle)

The Aufbau principle, or building-up principle, also called the Aufbau rule, states that in the ground state of an atom or ion, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels. For example, the 1s sub-shell is filled before the 2s sub-shell is occupied. In this way, the electrons of an atom or ion form the most stable electron configuration possible. An example is the configuration $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$ for the phosphorus atom, meaning that the 1s sub-shell has 2 electrons, and so on.

Salient Features of the Aufbau Principle

□According to the Aufbau principle, electrons first occupy those orbitals whose energy is the lowest. This implies that the electrons enter the orbitals having higher energies only when orbitals with lower energies have been completely filled.

$l = 0$ $l = 1$ $l = 2$ $l = 3$

n = 1

n = 2

n = 3

n = 4

n = 5

n = 6

n = 7

n = 8

1s

2s   2p

3s   3p   3d

4s   4p   4d   4f

5s   5p   5d   5f

6s   6p   6d

7s   7p

8s
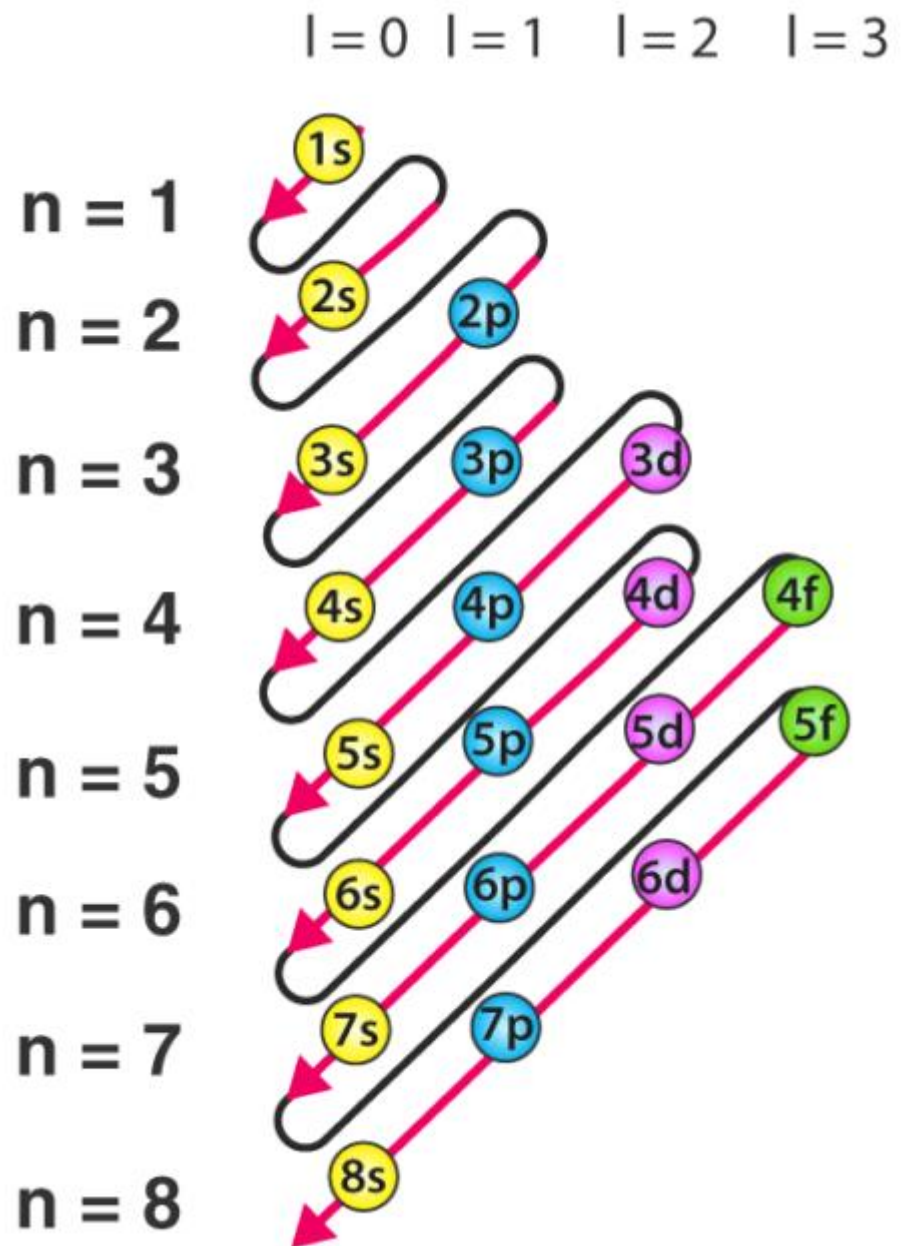
❑The order in which the energy of orbitals increases can be determined with the help of the (n+l) rule, where the sum of the principal and azimuthal quantum numbers determines the energy level of the orbital.

❑Lower (n+l) values correspond to lower orbital energies. If two orbitals share equal (n+l) values, the orbital with the lower n value is said to have lower energy associated with it.

❑The order in which the orbitals are filled with electrons is: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, and so on.
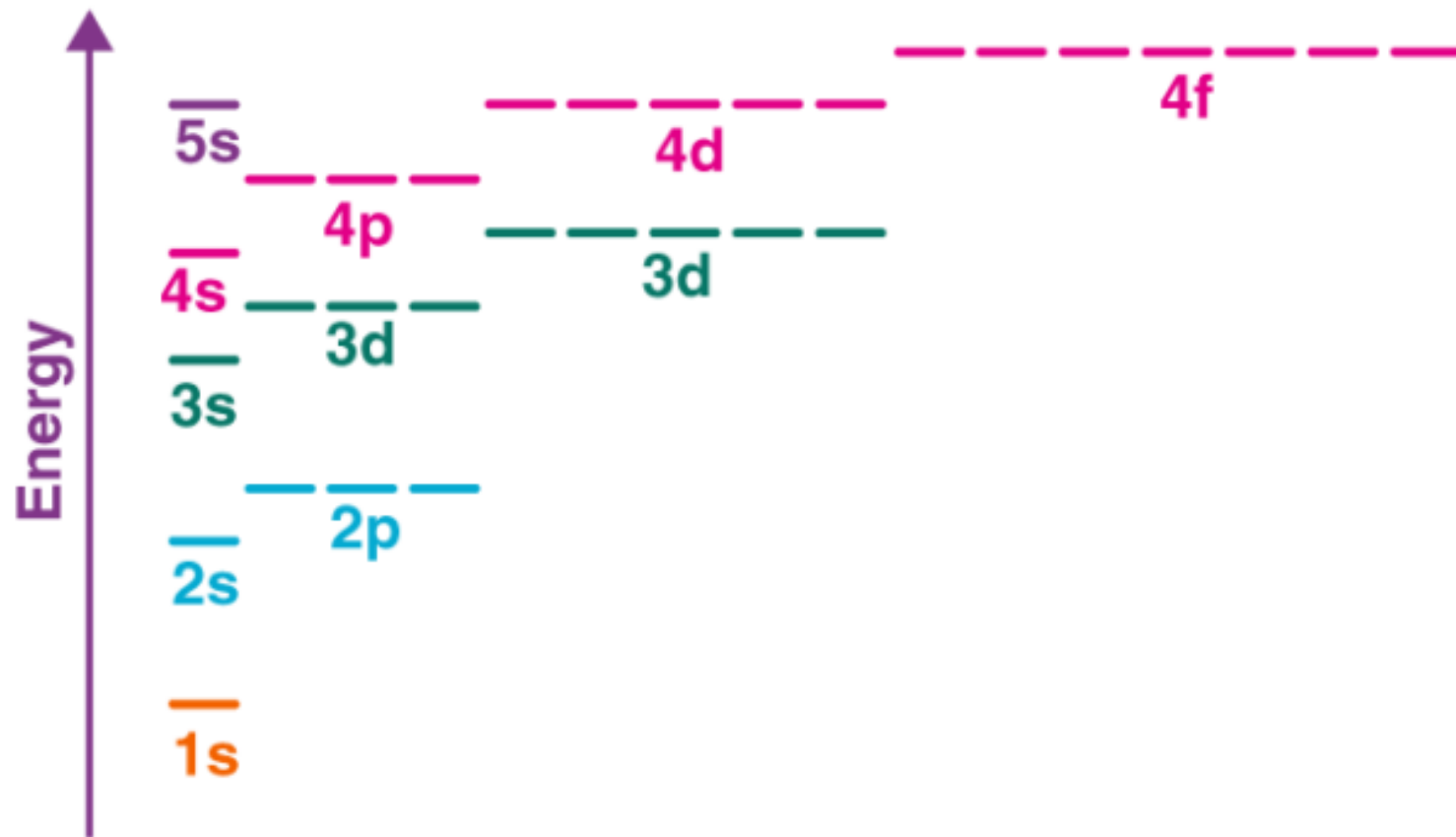
Fig. The energy gap between the different sub-shells is illustrated above.

Hund's Rule

When assigning electrons to orbitals, an electron first seeks to fill all the orbitals with similar energy before pairing with another electron in a half-filled orbital. Atoms at ground states tend to have as many unpaired electrons as possible. In visualizing this process, consider how electrons exhibit the same behavior as the same poles on a magnet would if they came into contact; as the negatively charged electrons fill orbitals, they first try to get as far as possible from each other before having to pair up.

Hund's rule states that
➢Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.
➢All of the electrons in singly occupied orbitals have the same spin (to maximize total spin).

According to Hund's Rule orbitals are filling up:
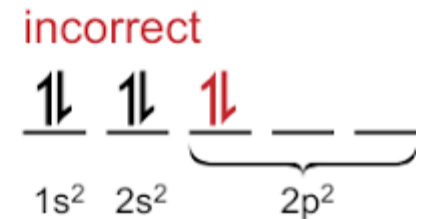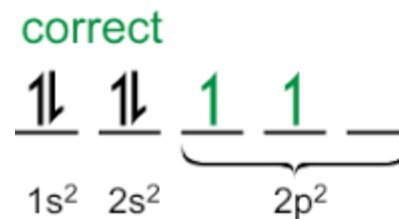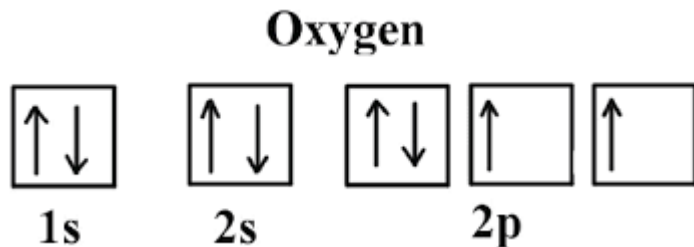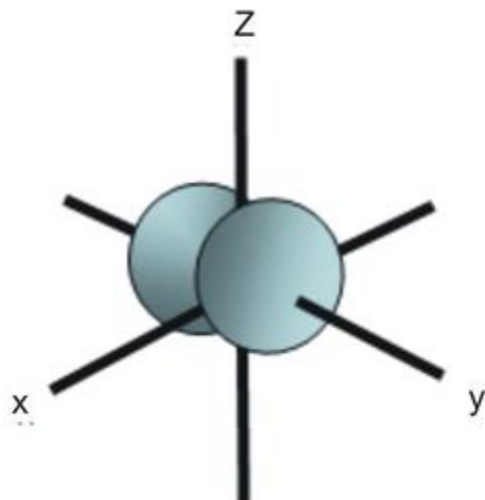
Atomic Orbitals

The three-dimensional region or space round the nucleus of an atom where there is maximum probability of finding an electron having a certain energy is called atomic orbital.
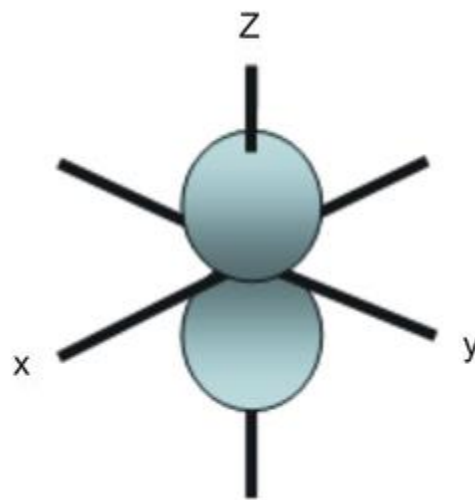
s-atomic orbital

An s orbital is spherically symmetric around the nucleus of the atom, like a hollow ball made of rather fluffy material with the nucleus at its centre. As the value of n for an energy level increases, the size of the s orbital increases.
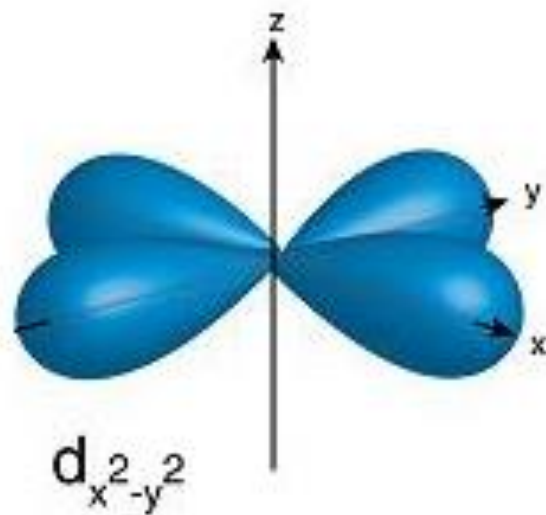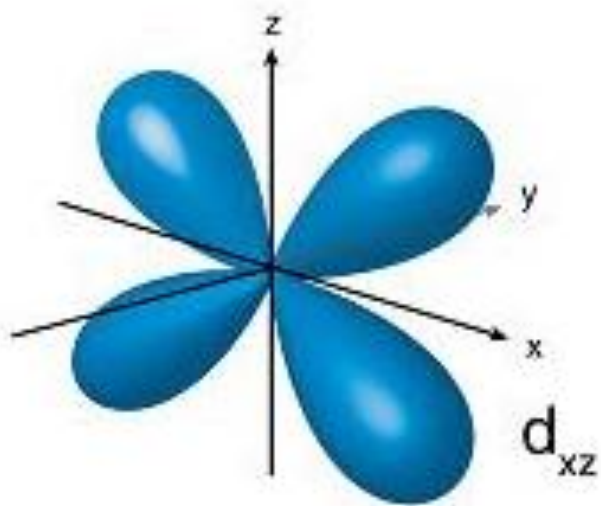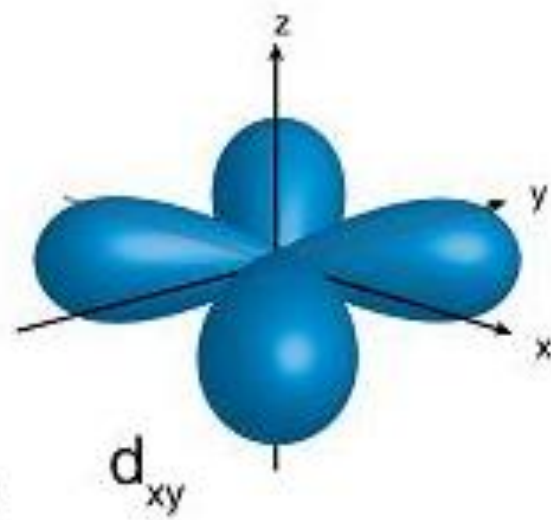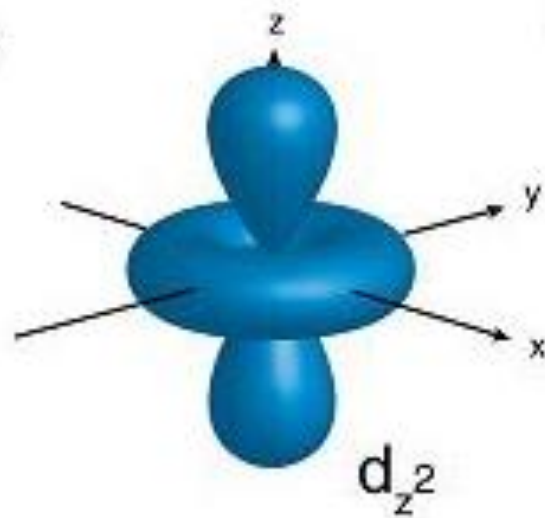
p_x p_y p_z
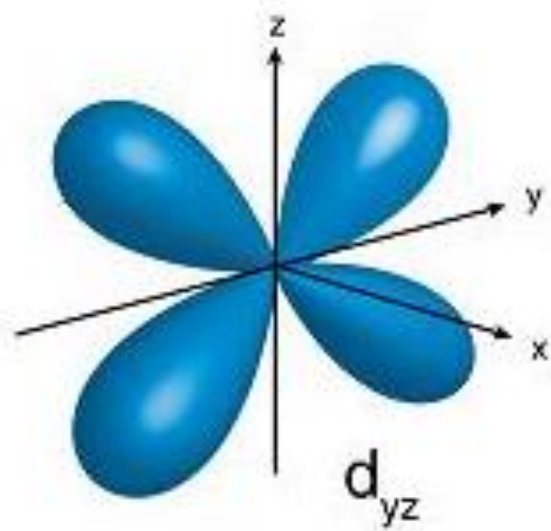
d_{yz}

d_{z^2}

d_{xy}

d_{xz}

$d_{x^2-y^2}$
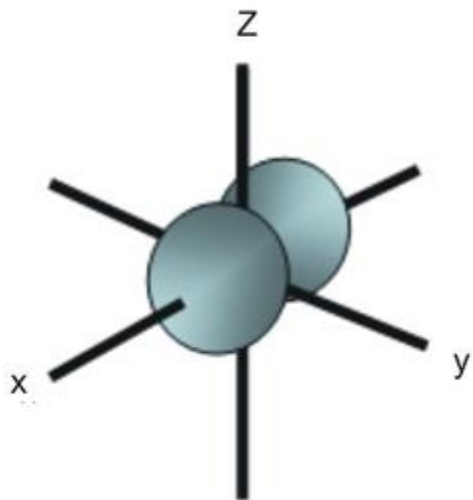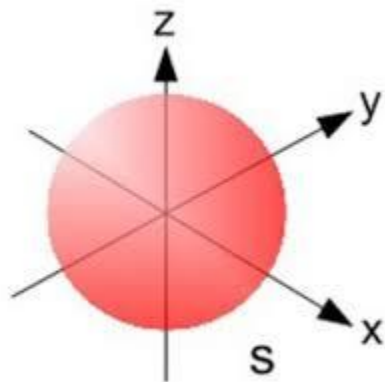
Electronic Configuration

The electron configuration of an element describes how electrons are distributed in its atomic orbitals. Electron configurations of atoms follow a standard notation in which all electron-containing atomic sub-shells are placed in a sequence. For example, the electron configuration of sodium is $1s^2 2s^2 2p^6 3s^1$. However, the standard notation often yields lengthy electron configurations. In such cases, an abbreviated or condensed notation may be used instead of the standard notation. In the abbreviated notation, the sequence of completely filled sub-shells that correspond to the electronic configuration of a noble

gas is replaced with the symbol of that noble gas in square brackets. Therefore, the abbreviated electron configuration of sodium is $[Ne]3s^1$ (the electron configuration of neon is $1s^2 2s^2 2p^6$, which can be abbreviated to $[He]2s^2 2p^6$).

Neon	$1s^2 2s^2 2p^6$		
Aluminum	$1s^2 2s^2 2p^6 3s^2 3p^1$	Becomes	$[Ne]\ 3s^2 3p^1$
Ar gon	$1s^2 2s^2 2p^6 3s^2 3p^6$		
Calcium	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	Becomes	$[Ar]\ 4s^2$