

### Ans to Qus. No - a

Explanation of Aufbau principle, Hund's rule and Pauli's exclusion principle with principle:

1) Aufbau Principle: In an atom, the electrons occupy different orbitals according to their increasing energy levels. That means electrons first fill up the more stable orbital of lowest energy and then gradually the orbitals of higher energy level.

Explanation:  $(n+l)$  rule for energy levels: The energy of different orbitals are calculated from the values of  $(n+l)$  of those orbitals.

Gradation of orbitals:  $1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p$  and  $6s$ .

Exception: Potassium (K) - (19)  $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 \boxed{3d^0 4s^1}$   
The last or 19<sup>th</sup> electron occupies  $4s$  orbital energy instead of higher energy  $3d$  orbital.

Pauli's exclusion Principle: The values of four quantum numbers of two electrons in an atom cannot be identical; at least one value must be different.

It means that ~~among~~ among the atom's electrons, one quantum number value ~~sho~~ must be different at least. For ex: there are 2 electrons in helium atom. The two electrons have the following values for four quantum numbers:

1st electron:  $n = 1, l = 0, m = 0, s = +\frac{1}{2}$

2nd electron:  $n = 1, l = 0, m = 0, s = -\frac{1}{2}$

Among the value of four quantum numbers of these two electrons, three values are identical but the fourth value is different. Hence Pauli ~~exclusion~~ exclusion principle is supported by helium atom.

Hund's Rule: The electron will distribute themselves in different degenerate orbitals in such a way that maximum number of electrons remain in unpaired state with spin of same direction. 'Degenerate orbitals' having same energy are three p-orbitals, five d-orbitals and seven f-orbitals. Hund's rule is not for s-orbital.

Example: The electronic configuration of N(7) =  $1s^2 2s^2 2p^3$ . In reality there are three 2p orbitals of same energy, which are designated as  $p_x, p_y, p_z$ . According to Hund's rule, here last three electrons will remain in three different p-orbitals with their spin in same direction.

Oxygen (O-8) =  $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

$$\begin{array}{ccc}
 1s^2 & 2s^2 & 2p \\
 = \uparrow\downarrow & \uparrow\downarrow & \begin{array}{ccc} x & y & z \\ \uparrow\downarrow & \uparrow & \uparrow \end{array}
 \end{array}$$

Exception: Copper (Cu-29):  ~~$1s^2$~~  [Ne]  $3s^2 3p^6 3d^{10} 4s^1$ . The last electron enters the 3d orbital instead of 4s orbital. Because  $3d^{10}$  is more stable than  $4s^1$ . But Hund's rule is not applicable for s-orbital. That's why it is an exception. Similarly as (Cr).

### Ans to Qus. No - b

Calculation of the total number of orbit and maximum electron containing capacity of 4th orbit calculating four quantum numbers.

Ans:- The total number of orbitals and electrons of 4th orbit are given below:

Principal Quantum Number	Subsidiary number (l)	Magnetic quantum number (m)	Spin quantum number (s)	Orbital	Total electron
4	0	0	$-\frac{1}{2}, +\frac{1}{2}$	1	2
	1	-1, 0, +1	$3(-\frac{1}{2}, +\frac{1}{2})$	3	6
	2	-2, -1, 0, +1, +2	$5(-\frac{1}{2}, +\frac{1}{2})$	5	10
	3	-3, -2, -1, 0, +1, +2, +3	$7(-\frac{1}{2}, +\frac{1}{2})$	7	14

$\therefore$  Total Number of Orbitals =  $(1 + 3 + 5 + 7) = 16$

Total Number of electron =  $(2 + 6 + 10 + 14) = 32$



## Ans to Qus. No - c

Shape of different orbitals: The shapes of different orbitals depend on the value of subshell or second quantum number ( $l$ ) and each subshell has a letter designation, such as with  $l=0$  called as s-orbital.  $l=1$  as p-orbital,  $l=2$  as d-orbital,  $l=3$  as f-orbital etc. of various possibilities, s, p, d, f orbitals are the most important because these are the most important because these are the only ones actually occupied in known elements. Let us look at each of the four individually.

1) Shape of s-Orbitals: All s-orbitals are spherical, meaning that the probability of finding s-electron depends only on distance from the nucleus, not on direction. Furthermore, because there is only one possible orientation of a sphere in space, an s orbital has  $m=0$  and there is only one s-orbital per shell. With the increase of the value of  $n$ , the size of s-orbital increases but density of electron cloud decreases, two electron cloud spheres are separated by a node having zero electron probability. All the s-orbitals are concentric.

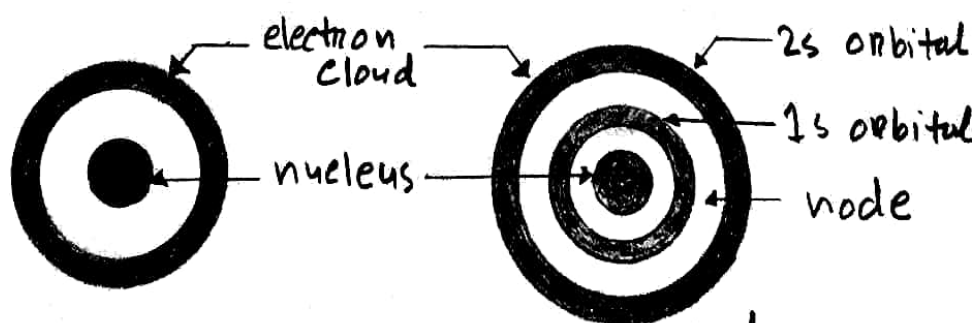
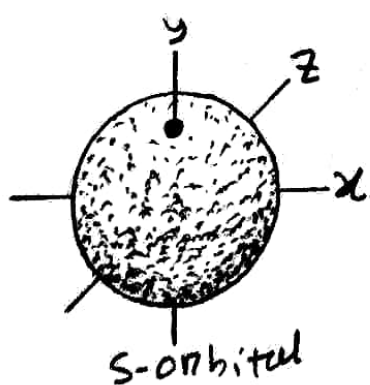


Fig : Shapes of s-orbitals.

Shape of p orbitals: From second shell or orbit where  $n=2$ , we get  $l=1$  (or p-orbital) and three possible values of  $m$  are  $-1, 0, +1$ . This means that there are three p-orbitals; they are  $p_x, p_y$  and  $p_z$  orbitals. They are identical in shape but they are situated along x-axis, y-axis and z-axis respectively and they are at right angles to each other. The shape of every p orbital is dumbbell shaped.

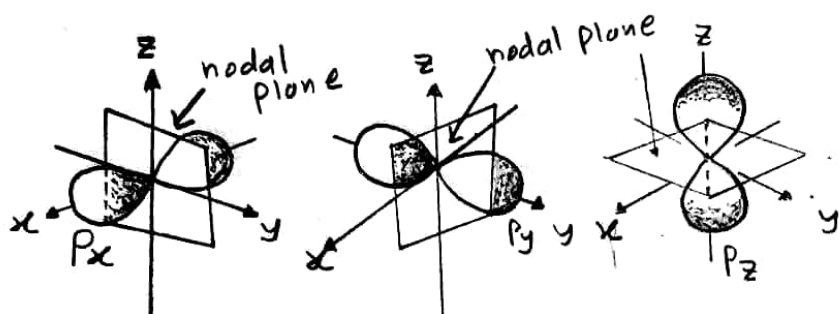


Fig: Shapes of three p-orbitals

3) Shape of d-orbitals: From third shell or orbit where  $n=3$ , we get  $l=2$  (or d-orbital) and five possible values for  $m$  are  $-2, -1, 0, +1, +2$ . This means that there are five different space orientations for d-orbitals, they are  $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}$  and  $d_{z^2}$  orbitals. The five d-orbitals are not identical in shapes.

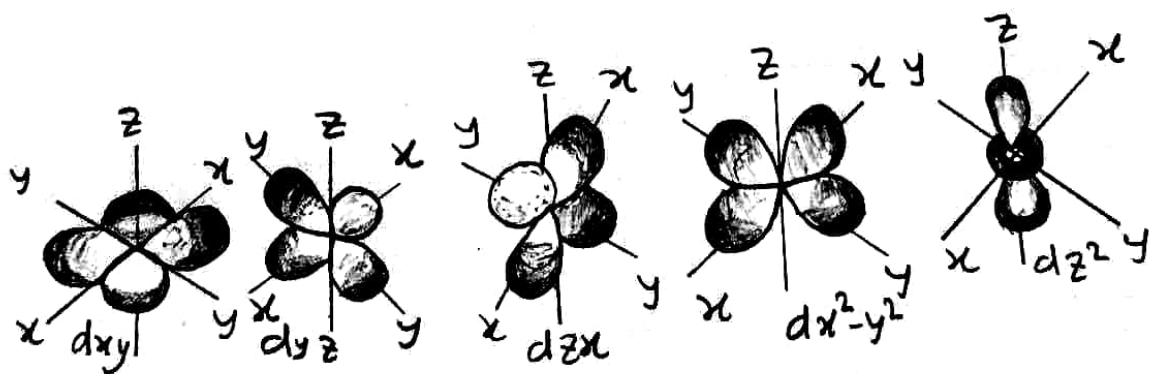


Fig: Shapes of five d-orbitals



The electrons in infinite number of excited hydrogen atoms in a sample absorb different amount of energy from same source and jump to different levels of higher energy. These states are unstable and so the electrons jump back to lower energy levels and thereby emit electromagnetic radiation of different energies and hence of different but definite frequencies.

When an electron jumps from different higher  $n_2$  energy level to lower  $n_1$  energy level, then the wave numbers ( $\bar{\nu}$ ) of emitted radiations are given by the following Rydberg equation:

$$\frac{1}{\lambda} = \bar{\nu} = R_H \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{ . Here } R_H \text{ is Rydberg constant } (1.09678 \times 10^7 \text{ m}^{-1})$$

- i) Lyman Series: when electron jumps from higher energy levels to 1st energy level.
- ii) Balmer Series: when electron jumps from higher energy levels to 2nd, ~~3rd, 4th and 5th~~ energy level.
- iii) Paschen Series: when electron jumps from higher energy level to 3rd energy level.
- iv) Brackett Series: when electron jumps from higher energy level to 4th energy level.
- v) Pfund Series: when electron jumps from higher energy level to 5th energy level.

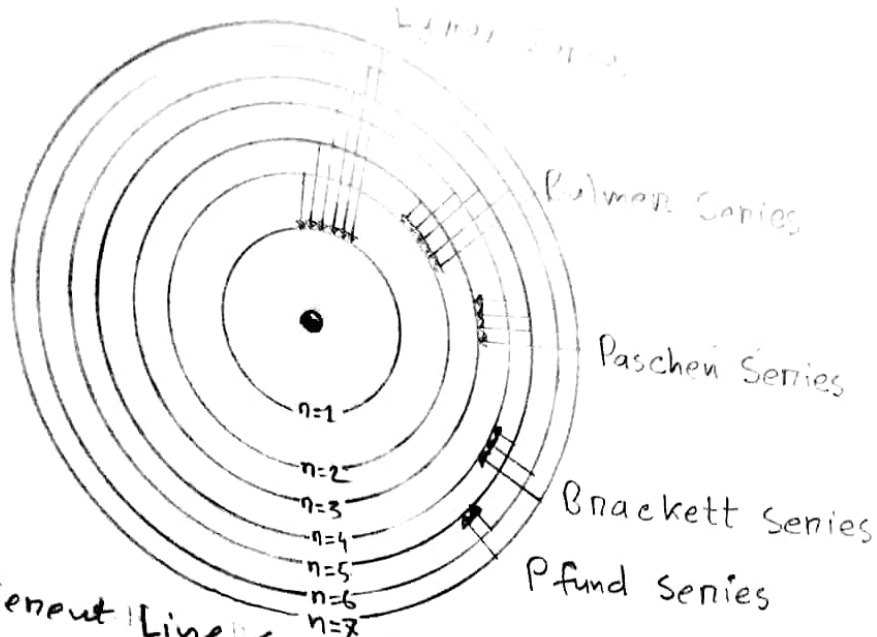


Fig: Different Line Spectrum of H-atoms from different regions

\* Lyman Series:  $n_1 = 1, n_2 = 2, 3, 4, 5, 6, 7, \dots \infty$

$$= (1.09678 \times 10^7) \times \left( \frac{1}{1^2} - \frac{1}{2^2} \right) = 8225850 \text{ m}^{-1}$$

$$= 8.22585 \times 10^6 \text{ m}^{-1}$$

\* Balmer Series:  $n_1 = 2, n_2 = 3, 4, 5, 6, 7, \dots \infty$

$$= (1.09678 \times 10^7) \times \left( \frac{1}{2^2} - \frac{1}{3^2} \right) = 1523305.9 \text{ m}^{-1}$$

$$= 1.52331 \times 10^6 \text{ m}^{-1}$$

\* Paschen Series:  $n_1 = 3, n_2 = 4, 5, 6, 7, \dots \infty$

$$= (1.09678 \times 10^7) \times \left( \frac{1}{3^2} - \frac{1}{4^2} \right) = 5.331569 \times 10^5 \text{ m}^{-1}$$

\* Brackett Series:  $n_1 = 4, n_2 = 5, 6, 7, \dots \infty$

$$= (1.09678 \times 10^7) \times \left( \frac{1}{4^2} - \frac{1}{5^2} \right) = 2.46775 \times 10^5 \text{ m}^{-1}$$

\* Pfund Series:  $n_1 = 5, n_2 = 6, 7, \dots \infty$

$$= (1.09678 \times 10^7) \times \left( \frac{1}{5^2} - \frac{1}{6^2} \right) = 1.340508 \times 10^5 \text{ m}^{-1}$$