MOLECULAR ORBITAL THEORY

1. ATOMIC ORBITALS (s,p,d,f) orbitals shape.
2. ELECTRONIC CONFIGURATION
3. MOLECULAR ORBITAL THEORY
   (BONDING & ANTIBONDING ORBITALS)
4. MOT DIAGRAMS OF HOMONUCLEAR& HETERONUCLEAR DIATOMIC MOLECULES

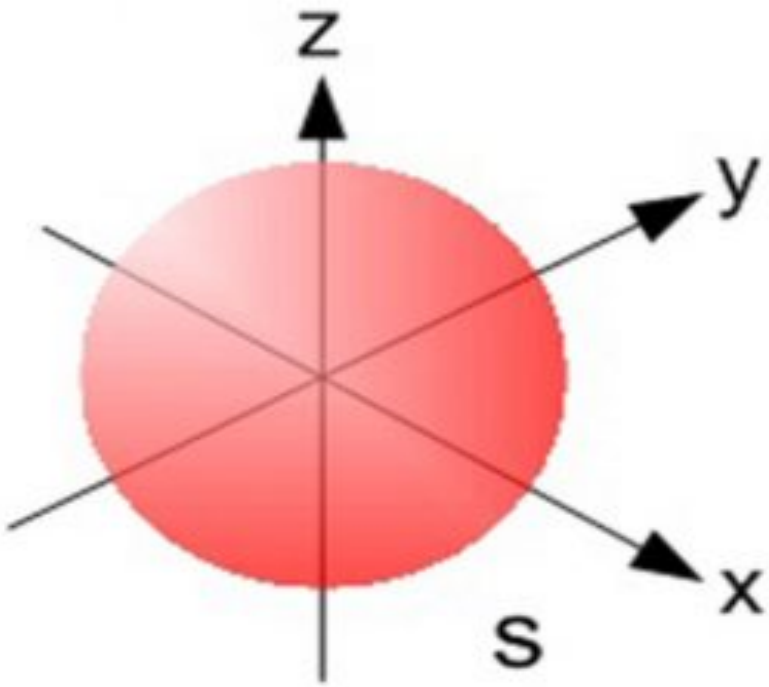
Be_2, O_2, CO, NO their bond order & magnetic properties

ATOMIC ORBITAL

- An **orbital** is the region of space around the nucleus within which the probability of finding an **electron** of given energy is maximum .

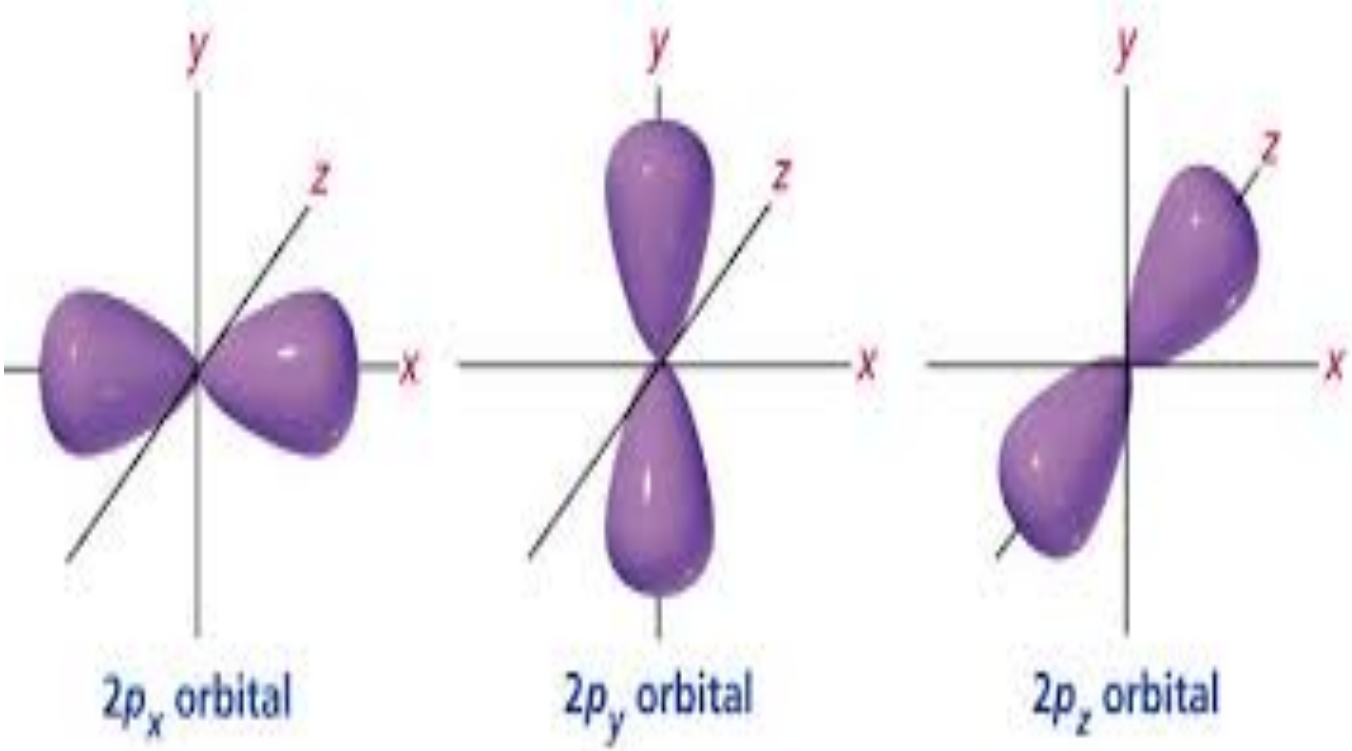
Atomic Orbitals

- S orbitals



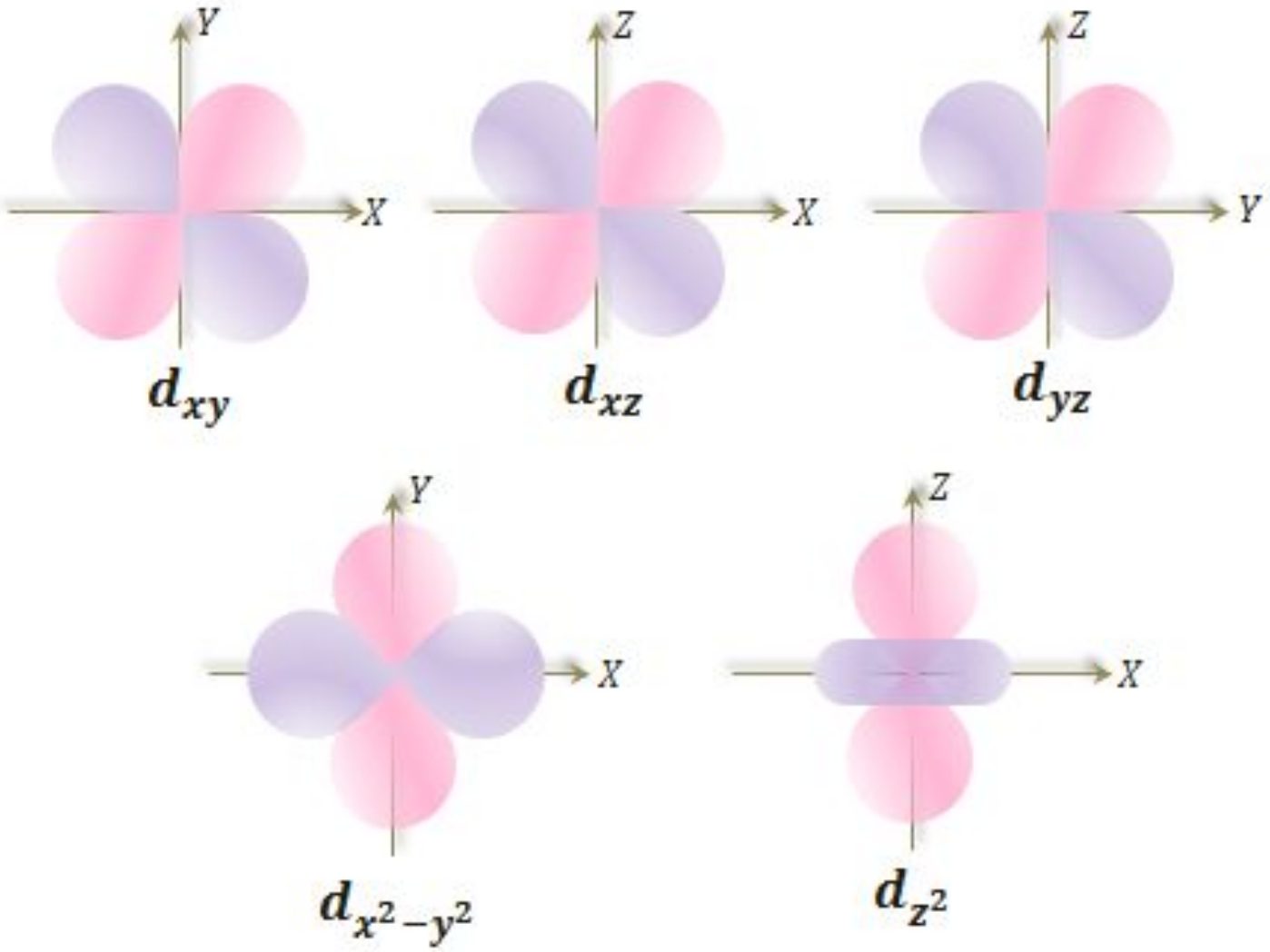
- For s-orbitals, when *l* = 0, the value of m is 0 i.e., there is only one possible orientation. This means that the probability of finding an electron is the same in all directions at a given distance from the nucleus. It should, therefore, be spherical in shape. Hence all s- orbitals are non- directional and spherically symmetrical about the nucleus.
- The size of an s-orbital depends upon value of the principal quantum number n. Greater the value of 'n' larger is the size of the orbital.

P orbitals



- or p-subshell *l* = 1, there are three values of m namely -1, 0, +1. It means that p orbitals can have three possible orientations. These three p-orbitals are equal in energy (degenerate state) but differ in their orientations. Each p-orbital consists of two lobes symmetrical about a particular axis. Depending upon the orientation of the lobes, these are denoted as $2p_x$, $2p_y$ and $2p_z$ accordingly as they are symmetrical about X,Y and Z - axis respectively.

d orbitals



- Magnetic **orbital** quantum number for **d orbitals** is given as (-2, -1, 0, 1, 2).
- It means d- orbitals can have five orientations. These are represented by d_{xy}, d_{yz}, d_{zx}, $d_{x}2_{-y}2$ and $d_{z}2$;. The d_{xy}, d_{yz} and d_{zx} orbitals have same shape i.e., clover leaf shape but they lie in XY, YZ and ZX-planes respectively.The d_{z2} orbital is symmetrical about Z-axis and has a dumb - bell shape with a doughnut shaped electron cloud in the centre. The d_{x2-y2} orbital is also clovar leaf shaped but its leaves are directed along the X and Y- axis.

QUIZ 1

- WRITE DIFFERENCE BETWEEN ORBIT & ORBITAL

ELECTRONIC CONFIGURATION

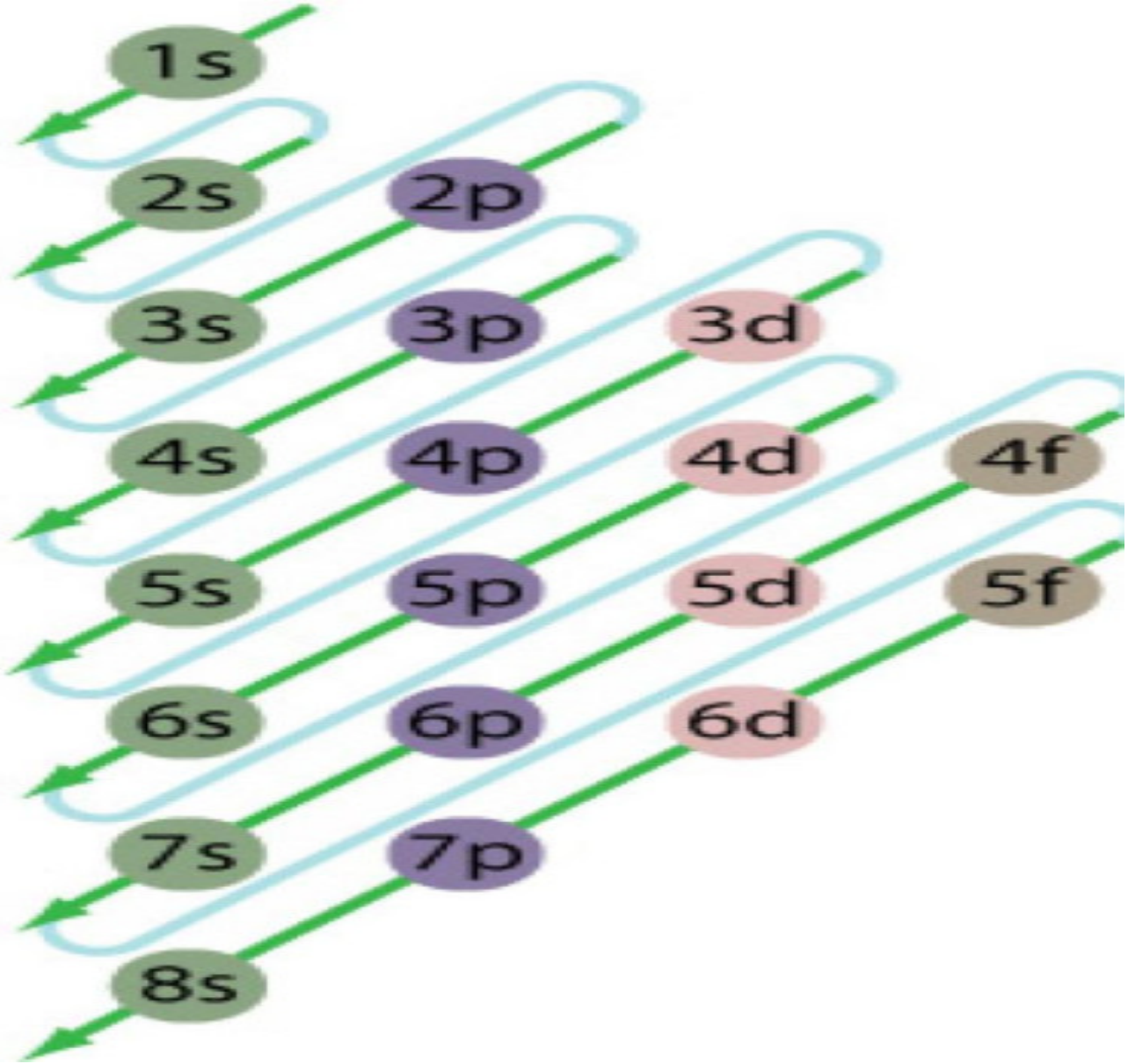
- The distribution of electrons in various orbitals is known as electronic configuration.

- **The filling of electrons in orbitas is determined by following rules.**

- 1) Aufbau Principle
- 2) Pauli's exclusion principle
- 3) Hund's Rule of maximum multiplicity

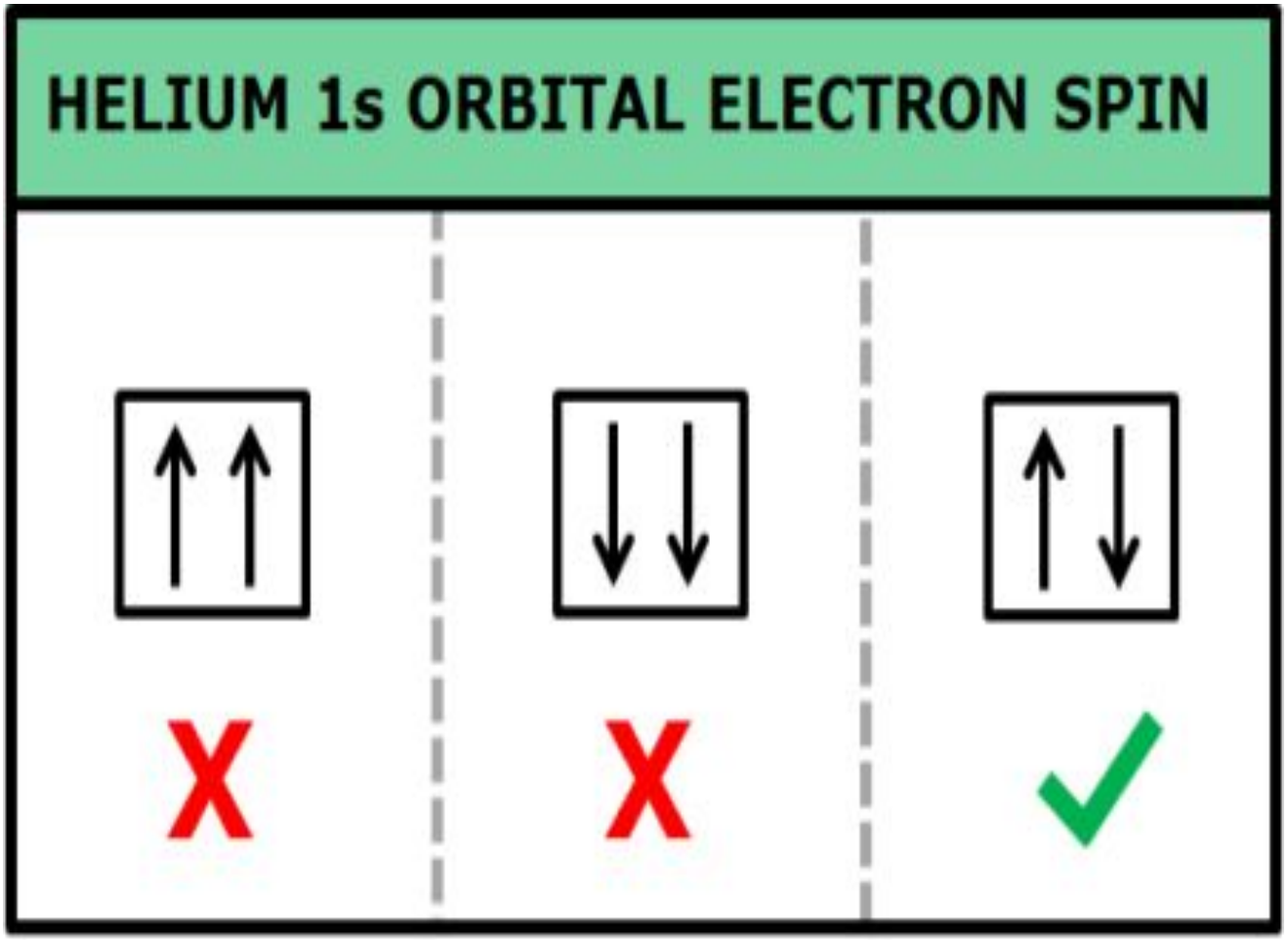
Aufbau Principle

- **The Building-Up (Aufbau) Principle**
- According to the principle, electrons fill orbitals starting at the lowest available energy states before filling higher states (e.g., 1s before 2s).


1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d
5f
6s
6p
6d
7s
7p
8s

- Following steps detail how to draw an Aufbau diagram:
- Determine the number of electrons that the atom has.
- Fill the s orbital in the first energy level (the 1s orbital) with the first two electrons.
- Fill the s orbital in the second energy level (the 2s orbital) with the second two electrons.
- Put one electron in each of the three p orbitals in the second energy level (the 2p orbitals) and then if there are still electrons remaining, go back and place a second electron in each of the 2p orbitals to complete the electron pairs.
- Continue in this way through each of the successive energy levels until all the electrons have been drawn.

PAULI'S EXCLUSION PRINCIPLE

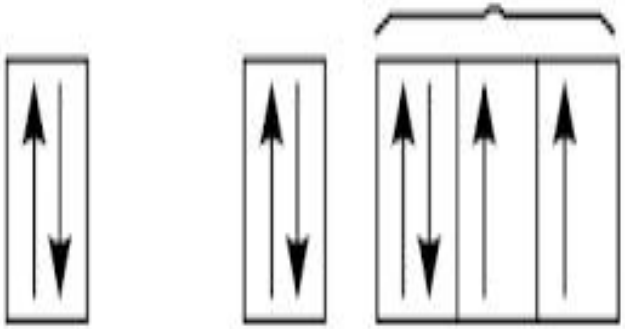


- **Pauli's Exclusion Principle**
- According to it: "no two electrons can have the same set of all four quantum numbers."
- Or, it states that an orbital can have maximum of two electrons and that must be of opposite spin. Due to this, it was concluded that an orbital can have maximum of two electrons which can have all 3-quantum number same but the spin will be definitely different.

Hund's Rule of Maximum Multiplicity

- When two or more orbitals of equal energy (or very close energy) are available, electrons will fill the orbitals singly before filling doubly. All the electrons in the orbitals will have the same spin to maximize the **multiplicity**.

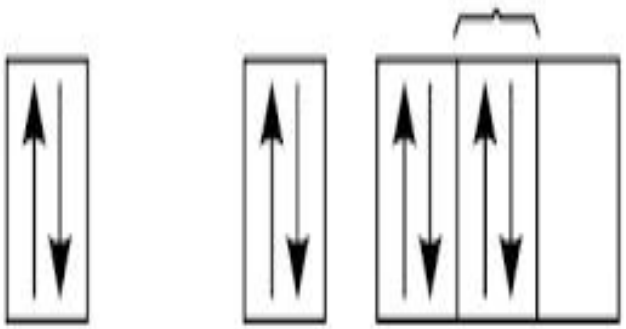
no electron-electron repulsion
equals lower energy



correct

or

electron-electron repulsion
equals higher energy



incorrect