

20/04/2021

Engineering ChemistryAtomic and Molecular structure - Tutorial

1) Give the main features of MOT.

Ans Features of MOT are as follows:

- 1) When two atoms approach each other, their atomic orbitals lose their identity and mutually overlap to form new orbitals called molecular orbitals.
- 2) The number of MO formed is equal to the number of overlapping atomic orbitals.
- 3) Maximum capacity of a MO is two electrons with opposite spins. MO is a polycentric region in space defined by its size and shape, associated with two or more atoms in a molecule and each has a capacity of two electrons with opposite spins.
- 4) The shape of MO formed depends on the type of combining atomic orbitals.
- 5) The bonding MO are represented by σ , π , δ etc whereas antibonding MO are represented by σ^* , π^* , δ^* etc.
- 6) Inner orbital MO which do not take part in bond formation are called non-bonding MO.

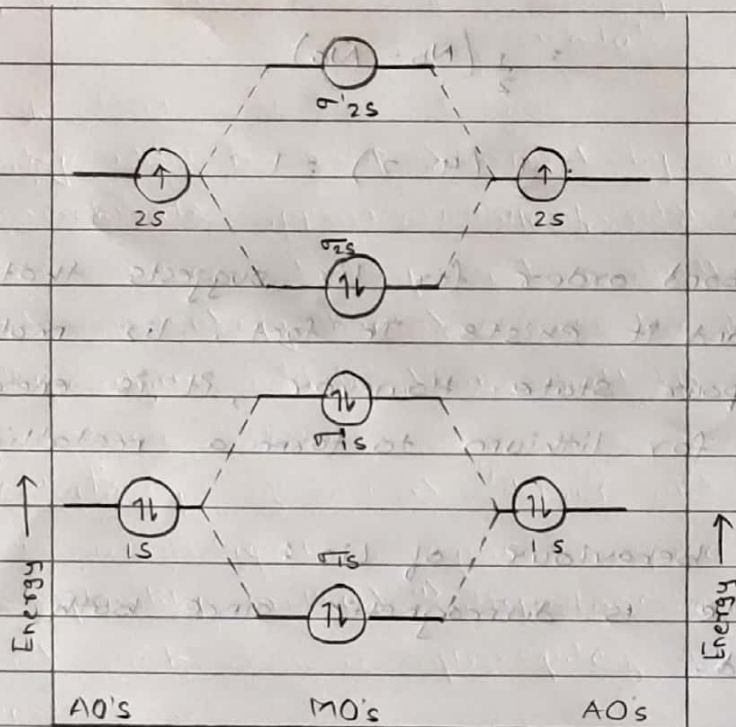
2) Distinguish between bonding and anti-bonding molecular orbital.

Ans

Bonding Molecular Orbitals	Anti-bonding Molecular orbitals.
<p>1) Formed by addition overlap of atomic orbitals.</p> <p>2) Possesses lower energy than that of the atomic orbitals.</p> <p>3) $\Psi_b = \Psi_A + \Psi_B$</p> <p>4) Imparts stability to the molecule</p> <p>5) Possesses high electron-density in the region between the two nuclei.</p> <p>6) It is formed when lobes of the combining atomic orbitals possesses same sign.</p>	<p>1) Formed by subtraction overlap of atomic orbitals.</p> <p>2) Possesses higher energy than that of atomic orbital.</p> <p>3) $\Psi_a = \Psi_A - \Psi_B$</p> <p>4) Imparts instability to the molecule</p> <p>5) Possesses low electron-density in the region between the two nuclei.</p> <p>6) It is formed when lobes of the combining atomic orbitals possesses opposite sign.</p>

3) With the help of MO energy level diagram explain formation of Lithium.

Ans



MO energy level diagram for Li_2

- 1) Lithium molecule is formed by the overlap of two lithium atoms each having the electronic configuration of $1s^2 2s^1$. So, there are total six electrons which have to be accommodated in 4 molecular orbitals viz σ_{1s} , σ_{1s}^* , σ_{2s} and σ_{2s}^* .
- 2) The six electrons are filled in these 4 molecular orbitals according to aufbau principle and Pauli's exclusion principle.
- 3) Hence, molecular orbital electronic configuration of Li_2 molecule = $\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 = \text{KK} \sigma_{2s}^2$.
- 4) Since, the inner shell of filled σ_{1s} and σ_{1s}^* molecular orbitals do not contribute to the bonding, and is written as KK which means K-shell is completely filled.

5) Bond order (Li_2) = $\frac{1}{2} [\text{Number of electrons in bonding molecular orbitals} - \text{Number of electrons in antibonding molecular orbitals}]$

$$= \frac{1}{2} (N_b - N_a)$$

$$= \frac{1}{2} (4 - 2) = 1$$

6) Positive bond order for Li_2 suggests that it is stable molecule and it exists. In fact, Li_2 molecule do exist in the vapour state. However, it is energetically more favourable for lithium to form a metallic structure in the solid.

7) Magnetic behaviour of Li_2 :

Li_2 molecule is diamagnetic since both the electrons are paired.