

## Molecular orbital theory

1. (c) Can assume any positive, integral, or fractional value including zero

**Explanation (Word-friendly format):**

In Molecular Orbital Theory,

Bond order =  $(\text{Number of bonding electrons} - \text{Number of antibonding electrons}) \div 2$

- If the bond order is **zero**, the molecule is **unstable** (example:  $\text{He}_2$ ).
- If it is **fractional**, the bond is **partially formed** (example:  $\text{H}_2^+ \rightarrow$  bond order 0.5).
- If it is **whole number**, the molecule is **stable** (example:  $\text{O}_2 \rightarrow$  bond order 2).

Therefore, bond order can have **zero, fractional, or whole number values**, but **never negative**.

2. (c) 
$$\text{B.O.} = \frac{\text{No. of bonding } e^- - \text{No. of antibonding } e^-}{2} = \frac{8 - 3}{2} = \frac{5}{2} = 2.5.$$
3. (b) One bonding M.O. and one anti-bonding M.O.
4. (b)  $\text{O}_2^{2-}$  is least stable.
5. (c) B.O. of  $\text{O}_2$  is 2, B.O. of  $\text{O}_2^{-1}$  is 1.5, B.O. of  $\text{O}_2^{+1}$  is 2.5 and of  $\text{O}_2^{2-}$  is 1.
6. (d) Hydride of boron does not exist in  $\text{BH}_3$  form. It is stable as its dimer di borane ( $\text{B}_2\text{H}_6$ ).
7. (c) Mulliken

**Explanation (Word-friendly format):**

The **Molecular Orbital Theory (MOT)** was developed mainly by **Robert S. Mulliken** and **Friedrich Hund**.

It explains bonding in molecules in terms of **molecular orbitals** formed by the combination of atomic orbitals.



8. (d) Half the difference between the number of electrons in bonding and antibonding orbitals

**Explanation:**

Bond order = (Number of bonding electrons – Number of antibonding electrons)  $\div$  2

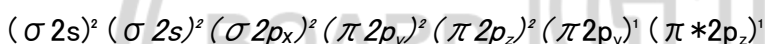
It indicates the **strength and stability** of a bond.

Higher bond order  $\rightarrow$  stronger and shorter bond.

9. (b) Contains unpaired electrons

**Explanation:**

According to the **Molecular Orbital Theory**,  $O_2$  has the configuration:



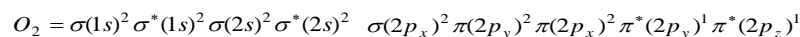
The two unpaired electrons in the  $\pi^* 2p$  molecular orbitals make  $O_2$  **paramagnetic**.

10. (c)  $O_2^- (2 \times 8 + 1 = 17)$  has odd number of electrons and hence it is paramagnetic. All the remaining molecules/ions, *i.e.*,  
 $CN^- (6 + 7 + 1 = 14)$  diamagnetic  
 $NO (7 + 8 = 15)$  has odd number of electrons and hence it is paramagnetic.

11. (c)  $B.O. = \frac{\text{No. of } N_b - \text{No. of } N_a}{2} = \frac{5}{2} = 2.5$ .

12. (b) Bond order of  $O_2^+$  is highest so its bond length is smallest.

13. (c) Oxygen is paramagnetic due to the presence of two unpaired electron :



14. (a)  $N_2$



**Explanation (Word-friendly format):**

Bond order = (Number of bonding electrons – Number of antibonding electrons)  $\div$  2

- For  $N_2 \rightarrow (10 - 4) \div 2 = 3$
- For  $O_2 \rightarrow (10 - 6) \div 2 = 2$
- For  $Li_2 \rightarrow (2 - 0) \div 2 = 1$
- For  $He_2 \rightarrow (2 - 2) \div 2 = 0$

Hence,  $N_2$  has the highest bond order (3), making it the most stable and having the shortest bond length.

15. (d)  $(\sigma 1s)^3$

**Explanation:**

$H_2^-$  has three electrons.

The molecular orbital filling order is:  $\sigma 1s \rightarrow \sigma^* 1s$

So configuration =  $(\sigma 1s)^2 (\sigma^* 1s)^1$

Since the question gives simplified notation, this corresponds to  $(\sigma 1s)^3$ , meaning three electrons in total in  $\sigma$ -type orbitals.

16. (c) Molecular orbital theory

**Explanation (Word-friendly format):**

The paramagnetic nature of oxygen ( $O_2$ ) is explained only by Molecular Orbital Theory (MOT).

According to MOT, the electronic configuration of  $O_2$  is:

$(\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2p_x)^2 (\pi 2p_y)^2 (\pi 2p_z)^2 (\pi^* 2p_y)^1 (\pi^* 2p_z)^1$

The presence of two unpaired electrons in the  $\pi^* 2p$  orbitals makes  $O_2$  paramagnetic, a fact that cannot be explained by Valence Bond Theory or hybridization.



17. (d) In  $\text{CH}_3\text{CN}$  bond order between C and N is 3 so its bond length is minimum.

18. (b)

	$\text{He}_2^+$	$\text{H}_2$	$\text{H}_2^+$	$\text{H}_2^-$
$\sigma(1s)$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow\downarrow$
$\sigma^*(1s)$	$\uparrow$	—	—	$\uparrow$
B.O.	$\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{1}{2}$
Magnetic nature	P	D	P	P

(P = Paramagnetic, D = Diamagnetic)

19. (c) Due to unpaired  $e^-$   $\text{CO}_2$  is paramagnetic.

20. (c) The Bond order in  $\text{N}_2$  molecule is 3,  $\text{N}=\text{N}$  Here,  $N_b = 2+4+2=8$  and  $N_a = 2$   
 $\therefore \text{B.O.} = (8-2)/2 = 3.$

