

Molecular orbital theory

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

Explanation (Word-friendly format):

In Molecular Orbital Theory,

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

- If the bond order is **zero**, the molecule is **unstable** (example: 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) $\text{B.O.} = \frac{\text{No. of bonding } e^- - \text{No. of antibondin } g e^-}{2} = \frac{8 - 3}{2} = \frac{5}{2} = 2.5 .$
3. (b) One bonding M.O. and one anti-bonding M.O.
4. (b) O_2^{2-} is least stable.
5. (c) B.O. of O_2 is 2, B.O. of O_2^{-1} is 1.5, B.O. of O_2^{+1} is 2.5 and of O_2^{2-} is 1.
6. (d) Hydride of boron does not exist in BH_3 form. It is stable as its dimer di borane (B_2H_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**, O₂ has the configuration:



The two unpaired electrons in the π^*2p molecular orbitals make O₂ paramagnetic.

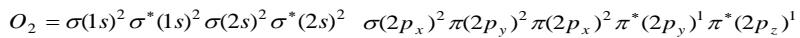
10. (c) O₂⁻ (2 × 8 + 1 = 17) has odd number of electrons and hence it is paramagnetic. All the remaining molecules/ions, i.e., CN⁻ (6 + 7 + 1 = 14) diamagnetic

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 O₂⁺ is highest so its bond length is smallest.

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



14. (a) N₂



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 σ -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 π^*2p orbitals makes O_2 paramagnetic, a fact that cannot be explained by Valence Bond Theory or hybridization.



17. (d) In CH_3CN bond order between C and N is 3 so its bond length is minimum.

18. (b)

	He_2^+	H_2	H_2^+	H_2^-
$\sigma(1s)$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	$\uparrow\downarrow$
$^*\sigma(1s)$	\uparrow	$\overline{\quad}$	$\overline{\quad}$	\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^- ClO_2 is paramagnetic.

20. (c) The Bond order in N_2 molecule is 3, $\pi \equiv \pi$. Here, $N_b = 2 + 4 + 2 = 8$ and $N_a = 2$
 \therefore B.O. = $(8 - 2)/2 = 3$.

