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 = (Number of bonding electrons − Number of antibonding electrons) ÷ 2

- If the bond order is **zero**, the molecule is **unstable** (example: He_2).
- If it is **fractional**, the bond is **partially formed** (example: H_2^+ → bond order 0.5).
- If it is **whole number**, the molecule is **stable** (example: O_2 → 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) 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) ÷ 2
It indicates the **strength and stability** of a bond.
Higher bond order → stronger and shorter bond.

9. **(b) Contains unpaired electrons**

Explanation:
According to the **Molecular Orbital Theory**, O_2 has the configuration:
$(\sigma 2s)^2 (\sigma 2s)^2 (\sigma 2p_x)^2 (\pi 2p_y)^2 (\pi 2p_z)^2 (\pi 2p_y)^1 (\pi *2p_z)^1$

The two unpaired electrons in the **π*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) $\text{B.O.} = \dfrac{\text{No. of } N_b - \text{No. of } N_a}{2} = \dfrac{5}{2} = 2.5$.

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 :
$O_2 = \sigma(1s)^2 \sigma^*(1s)^2 \sigma(2s)^2 \sigma^*(2s)^2 \quad \sigma(2p_x)^2 \pi(2p_y)^2 \pi(2p_x)^2 \pi^*(2p_y)^1 \pi^*(2p_z)^1$

14. **(a) N_2**

Explanation (Word-friendly format):
Bond order = (Number of bonding electrons − Number of antibonding electrons) ÷ 2

- For N_2 → (10 − 4) ÷ 2 = **3**
- For O_2 → (10 − 6) ÷ 2 = **2**
- For Li_2 → (2 − 0) ÷ 2 = **1**
- For He_2 → (2 − 2) ÷ 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^-
$\sigma(1s)$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow\downarrow$
$\overset{*}{\sigma}(1s)$	$\uparrow$	—	—	$\uparrow$
$B.O.$	$\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{1}{2}$
Magnetic nature	P	D	P	P

(P = Paramagnetic, D = Diamagnetic)

19. (c) Due to unpaired e^- ClO_2 is paramagnetic.

20. (c) The Bond order in N_2 molecule is 3, $N \equiv N$ Here, $N_b = 2 + 4 + 2 = 8$ and $N_a = 2$

$\therefore$ B.O. $= (8 - 2)/2 = 3$.