Molecular Orbital Model

Bond Order = $\frac{\text{number of bonding electrons} - \text{number of antibonding electrons}}{2}$

Paramagnetic = has unpaired electrons, is attracted to a magnetic field

Diamagnetic = does not have unpaired electrons, repelled by a magnetic field

1. Fill in MO diagrams for the following diatomics. Determine their bond order and whether they are paramagnetic or diamagnetic.

A. O_2 z = 8
B. O_2^+ z = 8
C. C_2 z = 6
D. C_2^- z = 6
E. F_2 z = 9
F. N_2^+ z = 7
G. N_2 z = 7

2. Which has a shorter bond, O_2 or O_2^+ ?

3. Which has a greater bond strength, C_2 or C_2^-?

4. Which has a longer bond, N_2 or N_2^+?

Bond order $O_2 = \frac{8-4}{2} = 2$

$O_2^+ = \frac{8-3}{2} = \frac{5}{2} = 2.5$ ← higher BO ⇒ shorter BL

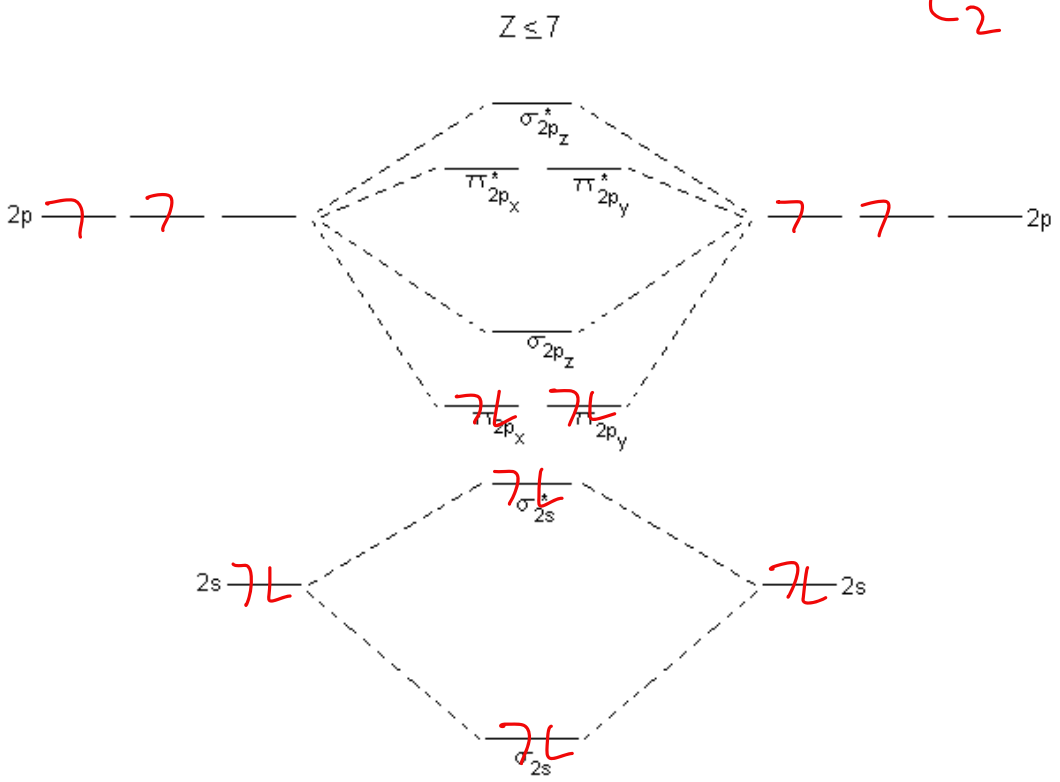
Bond order $C_2 = \frac{6-2}{2} = 2$

$C_2^- = \frac{7-2}{2} = 2.5$ ← higher BO ⇒ greater BS

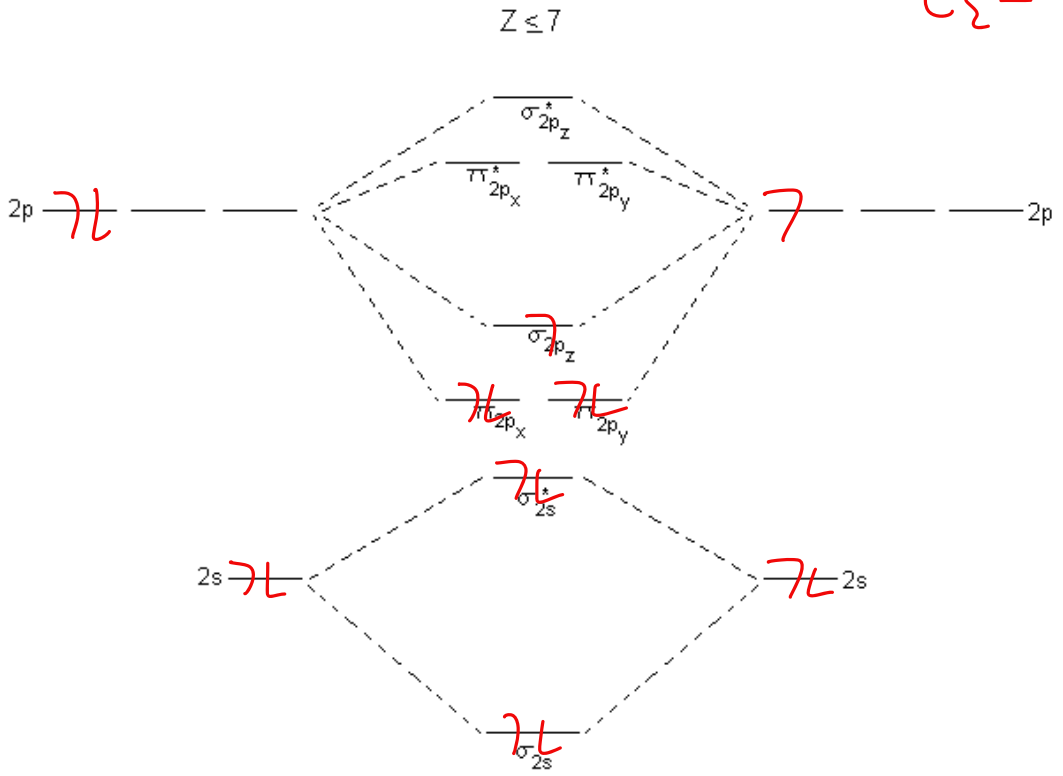
Bond order $N_2^+ = \frac{7-2}{2} = 2.5$ ← smaller BO ⇒ longer BL

$N_2 = \frac{8-2}{2} = 3$

C_2 $2 \times 4 = 8 e^-s$

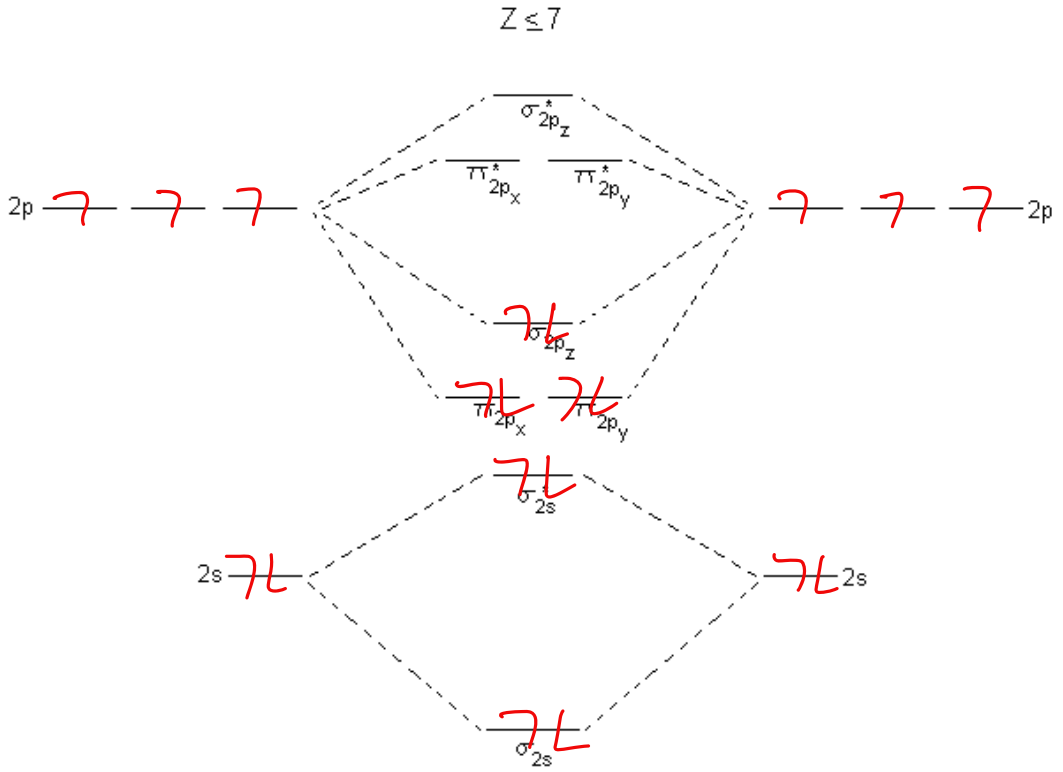


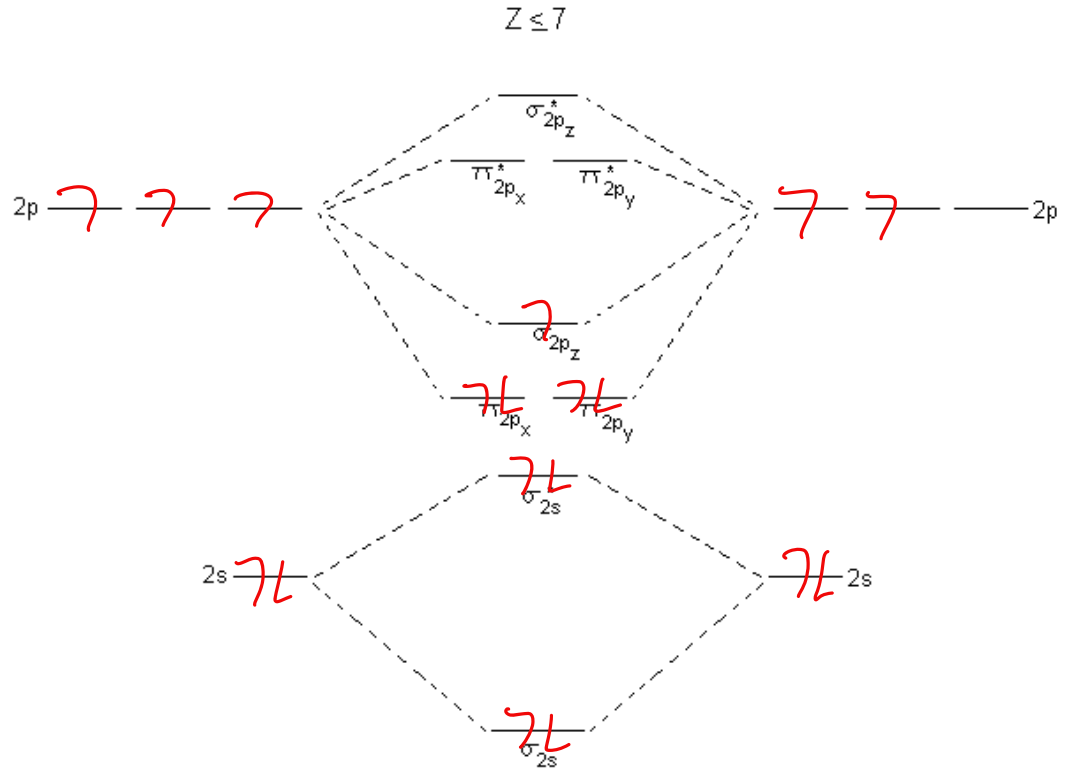
C_2 — 8 e⁻'s



N_2

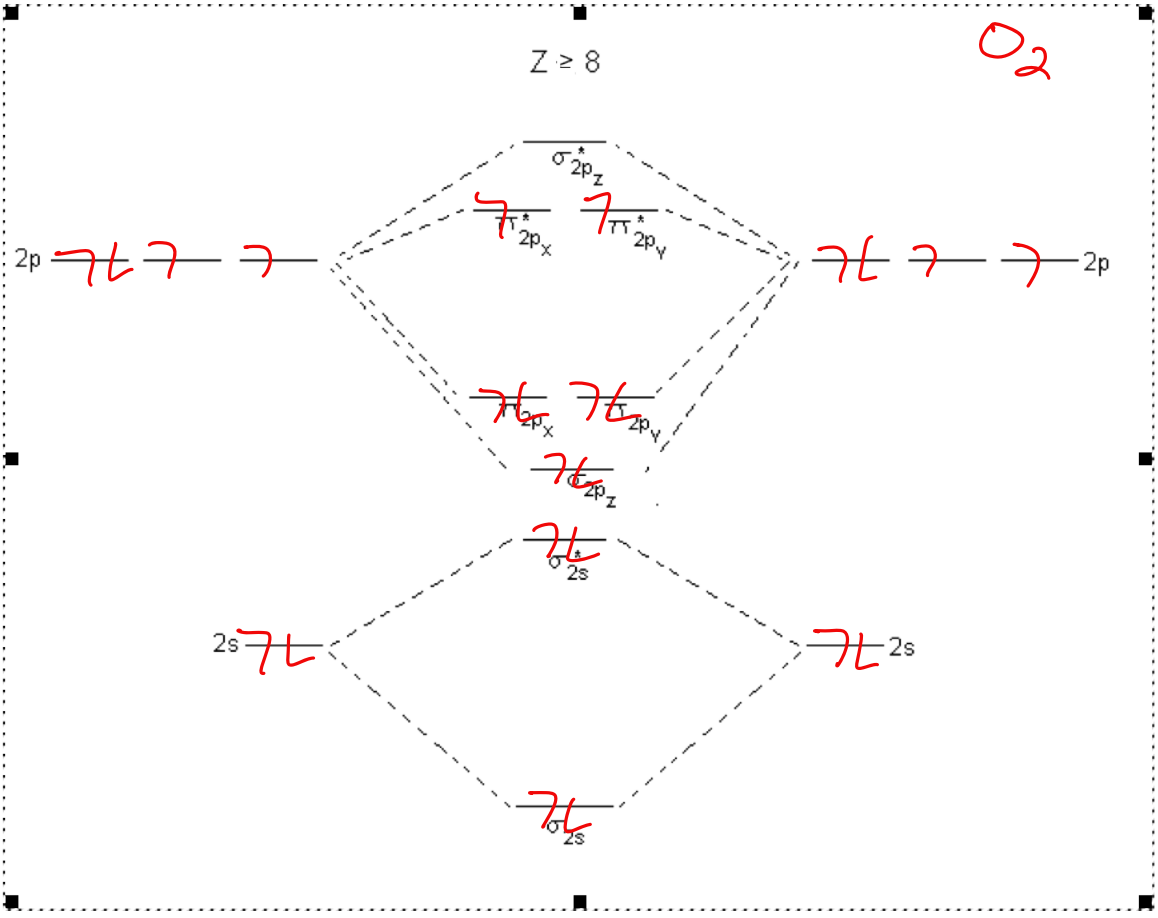
2 x 5 = 10





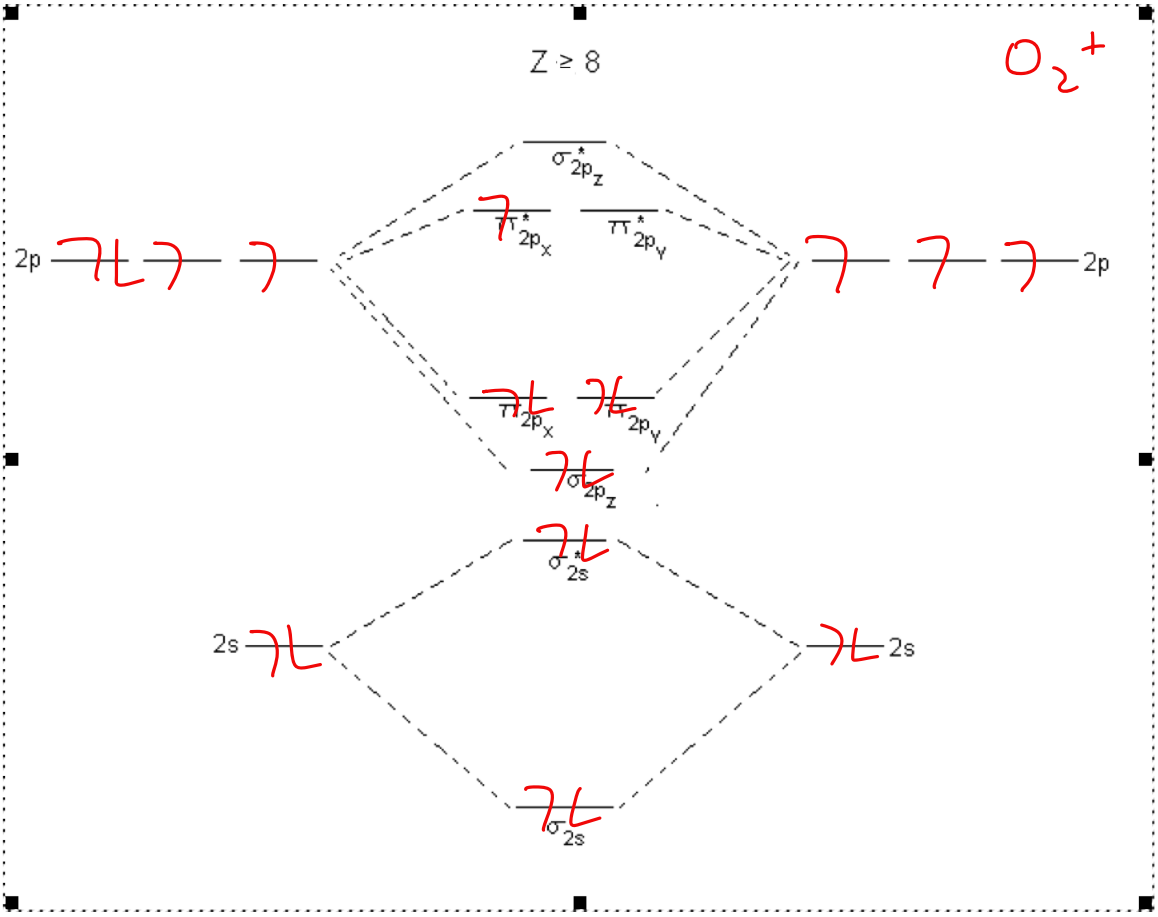
N_2^+

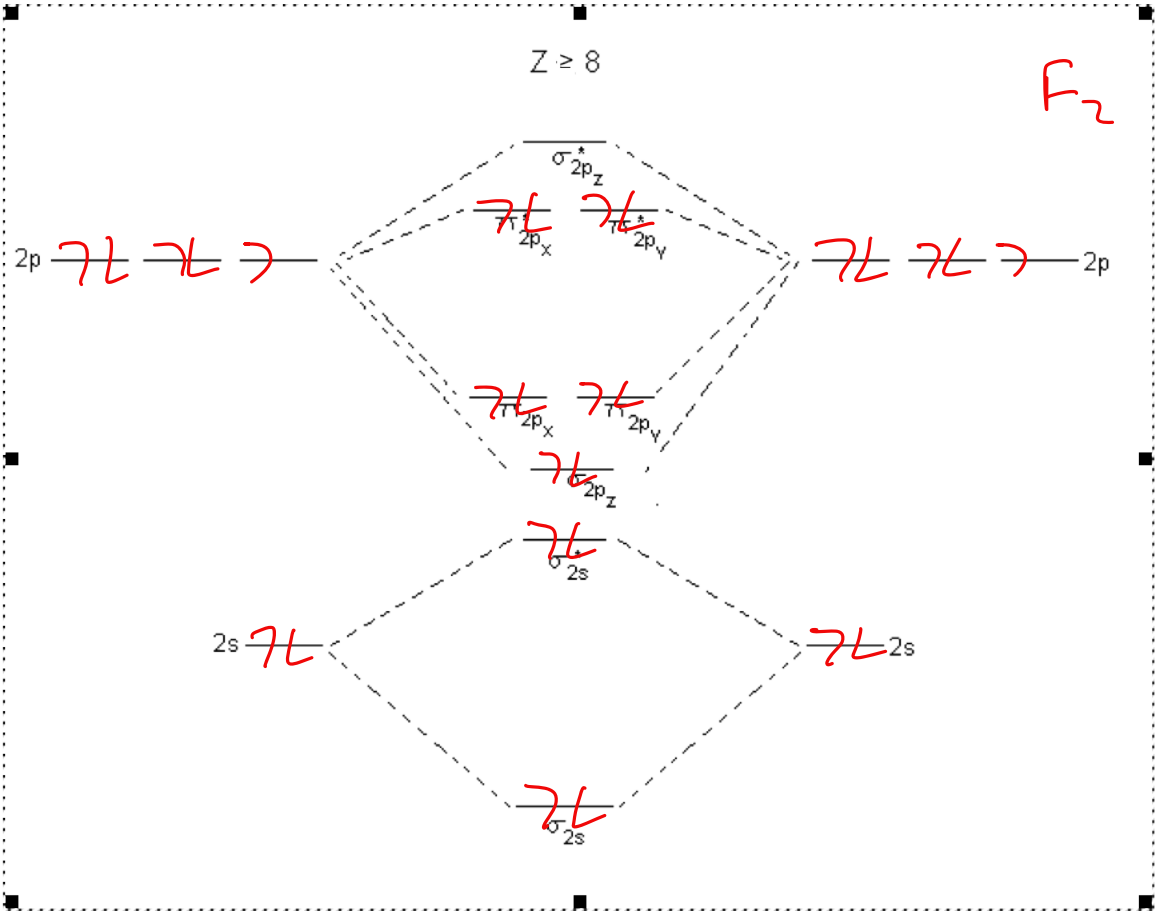
$2 \times 5 - 1 = 9$

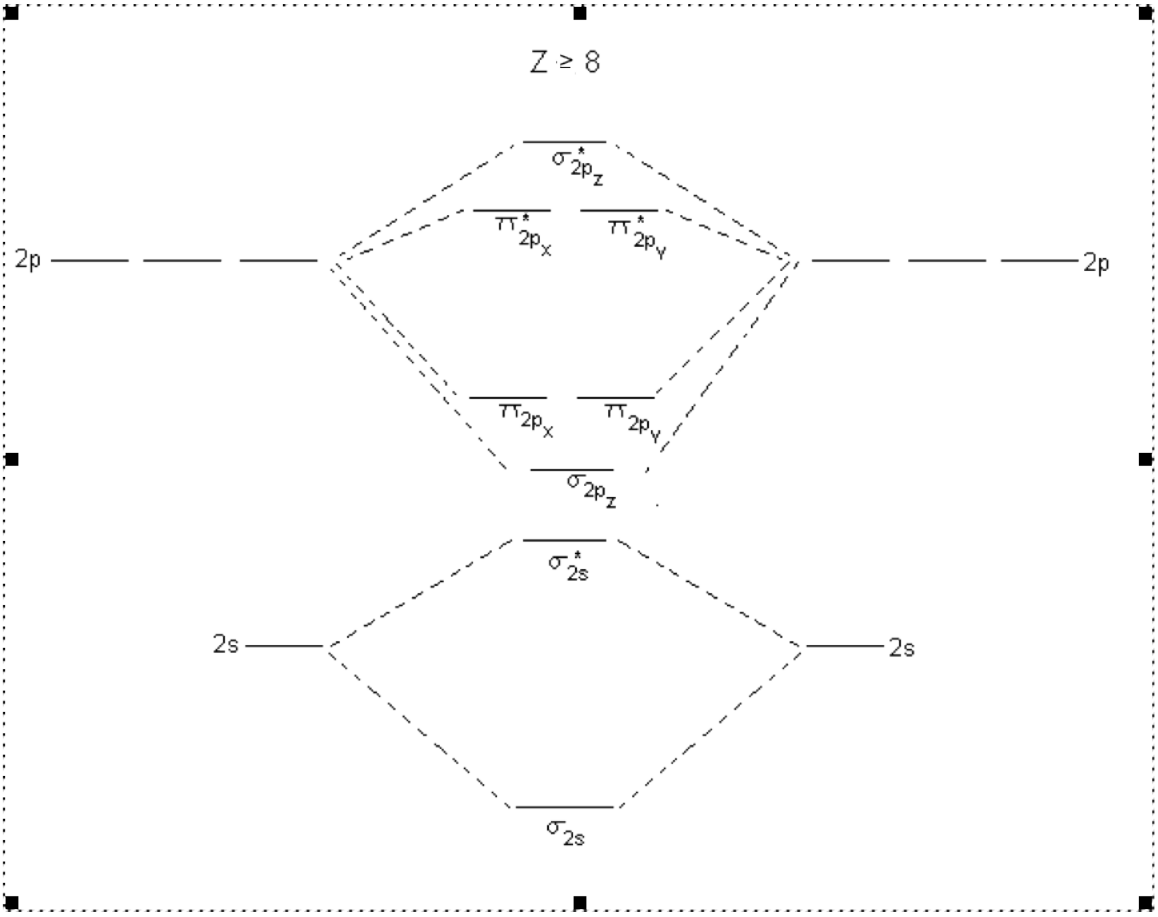


O_2

$2 \times 6 e^- -$


Z ≥ 8
O_2^+
2×6 = 12
−1 = 11
$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$
$\pi^*_{2p_y}$
2p
2p
π_{2p_x}
π_{2p_y}
σ_{2p_z}
σ^*_{2s}
2s
2s
σ_{2s}


Z ≥ 8
F_2
2×7 = 14
$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$
$\pi^*_{2p_y}$
2p
2p
π_{2p_x}
π_{2p_y}
σ_{2p_z}
σ^*_{2s}
2s
2s
σ_{2s}


Z ≥ 8
$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$
$\pi^*_{2p_y}$
2p
2p
π_{2p_x}
π_{2p_y}
σ_{2p_z}
σ^*_{2s}
2s
2s
σ_{2s}