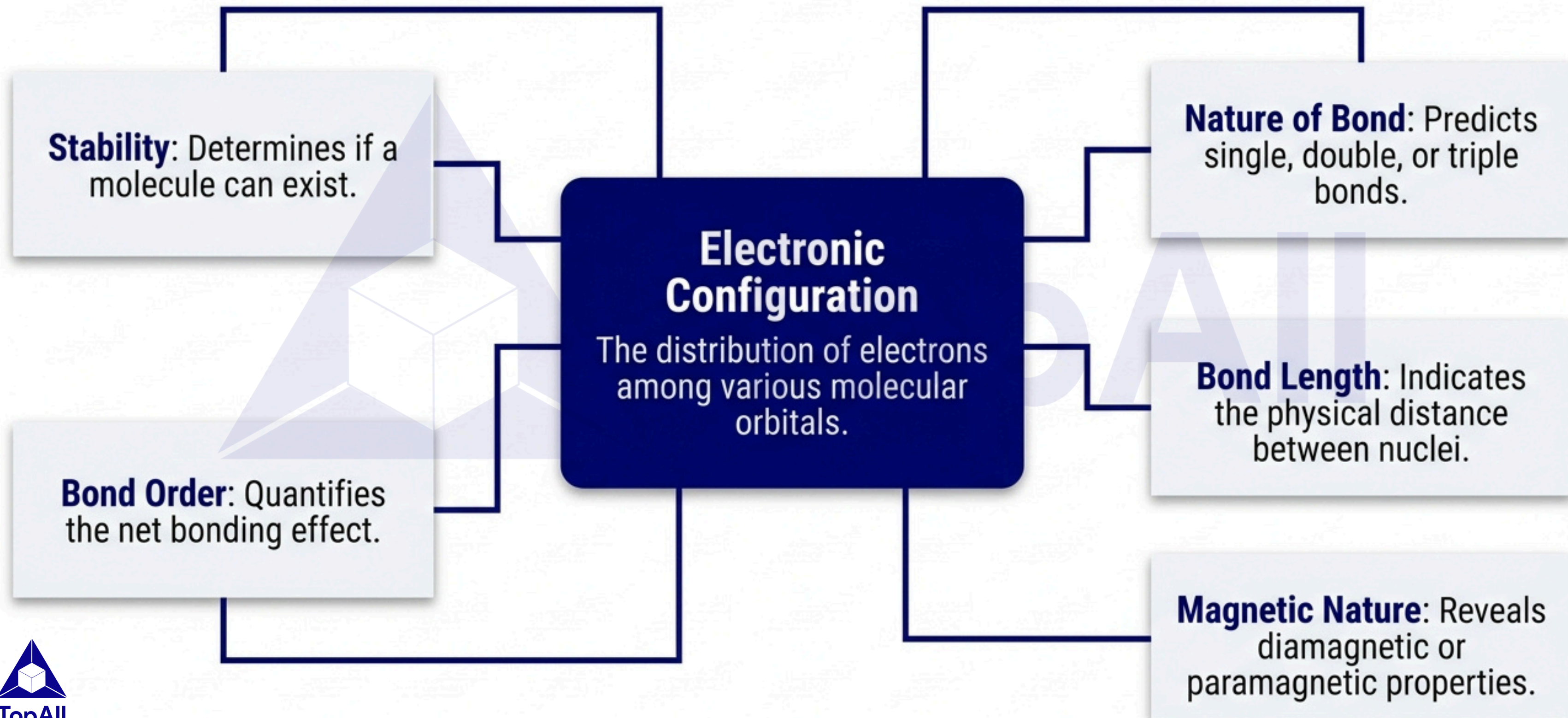


The Molecular Blueprint: What MO Configuration Predicts



The Stability Threshold: Bonding vs. Antibonding

The Variables

N_b

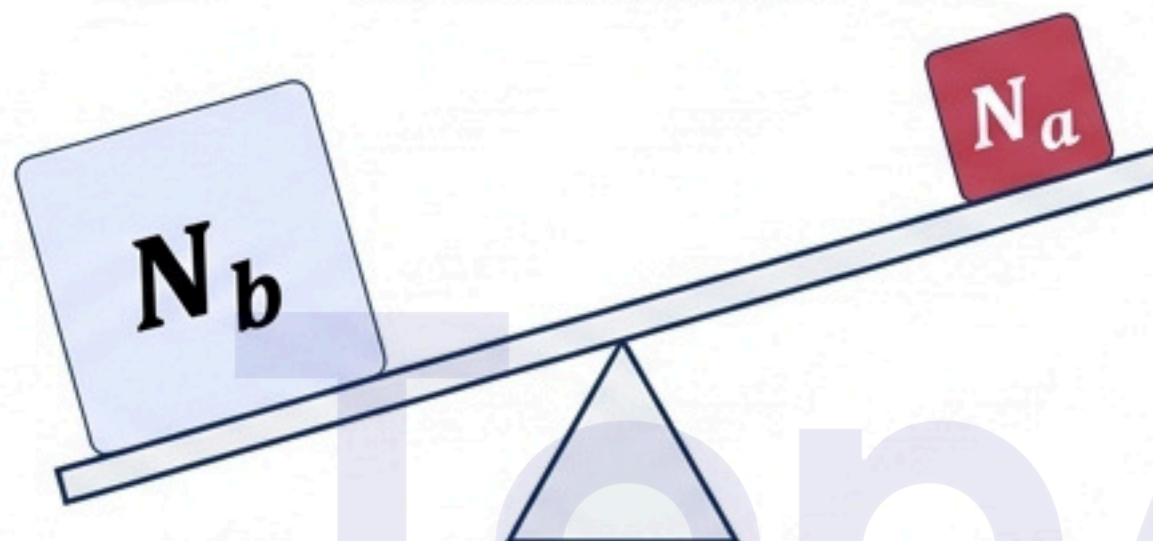
Number of electrons in
bonding orbitals
(Stabilizing influence)

N_a

Number of electrons in
antibonding orbitals
(Destabilizing influence)

The Outcomes

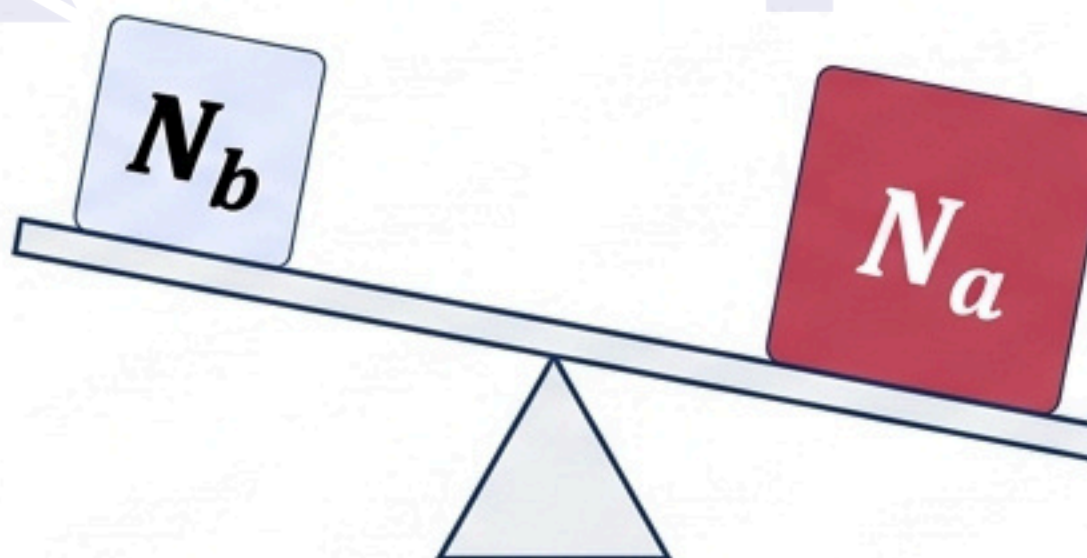
Stable Molecule



$$N_b > N_a$$

More bonding orbitals
occupied; bonding
influence is stronger.

Unstable Molecule



$$N_b < N_a \text{ OR } N_b = N_a$$

Antibonding influence
overcomes or neutralizes
bonding.

Calculating Bond Order (B.O.)



Bond Order: One half the difference between bonding and antibonding electrons.

The Pair Factor: Accounts for the fact that two electrons make up a single chemical bond.

Net Bonding Electrons: The surplus of stabilizing electrons over destabilizing ones.

The diagram shows the formula for Bond Order (B.O.) with arrows pointing to its parts: "B.O." is pointed to by the "Bond Order" definition; the fraction $\frac{1}{2}$ is pointed to by the "Pair Factor" definition; and the expression $(N_b - N_a)$ is pointed to by the "Net Bonding Electrons" definition. A large, faint "TopAll" watermark is visible in the background.

$$\text{B.O.} = \frac{1}{2} (N_b - N_a)$$

The Rules

Positive B.O. =
Stable molecule.

Negative or Zero B.O. =
Unstable molecule.

Integral Values (1, 2, or 3)
correspond directly to single,
double, or triple bonds.



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$$E=mc^2$$



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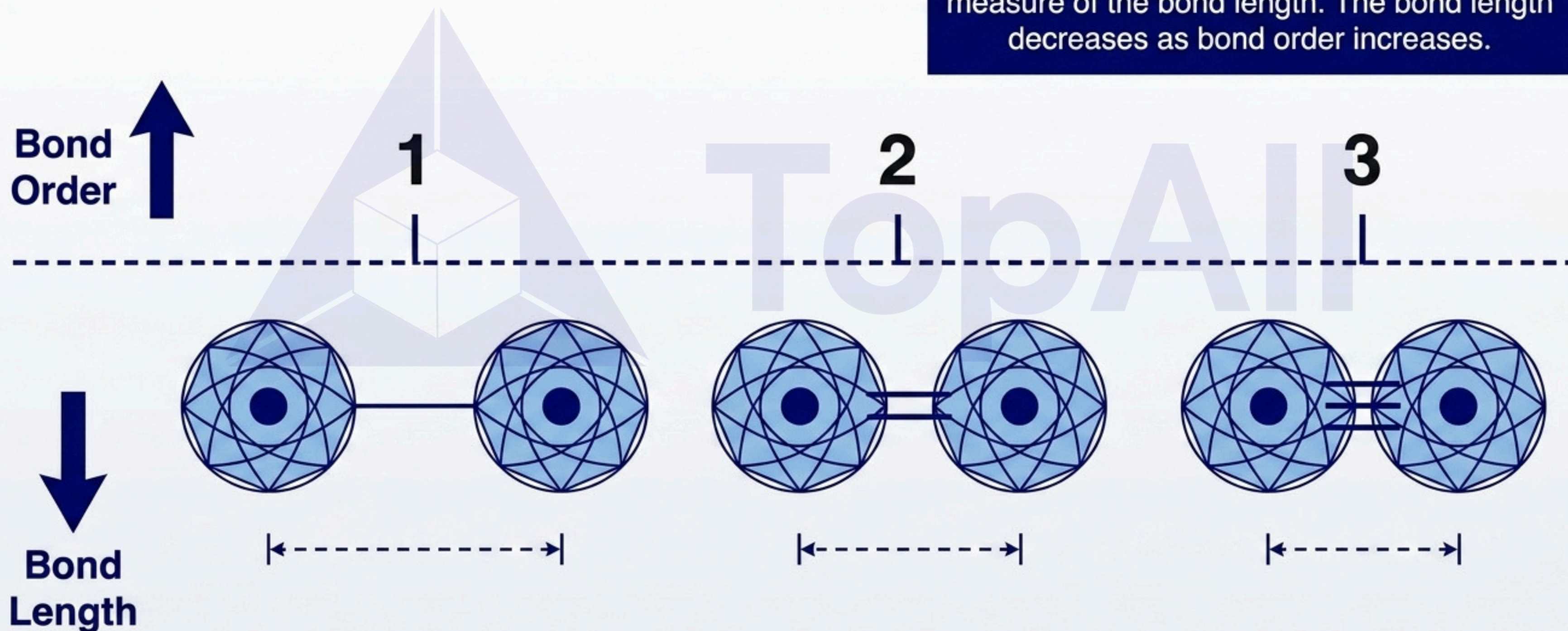
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- » Climb the Leaderboard Among Fellow Aspirants
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- » Get Clear Explanations, Not Just Marks
- » Track Your Performance Smarter



The Inverse Relationship: Order vs. Length

The bond order between two atoms in a molecule may be taken as an approximate measure of the bond length. The bond length decreases as bond order increases.



Magnetic Diagnostics: Paired vs. Unpaired

Diamagnetic

Definition: Repelled by a magnetic field.

Condition: All molecular orbitals are doubly occupied (paired).



Paramagnetic

Definition: Attracted by a magnetic field.

Condition: One or more molecular orbitals are singly occupied (unpaired).



The Oxygen (O_2) molecule is a classic paramagnetic example.

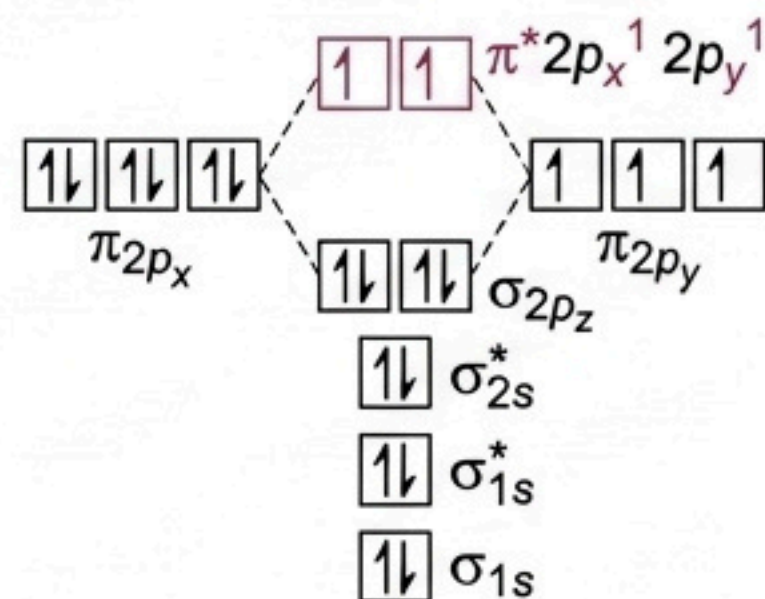
Analytical Workflow: The Oxygen (O_2) Example

Step 1: Total Electrons

Oxygen atom = $8 e^-$.
Therefore,
 $O_2 = 16 e^-$.

Step 2: Fill Molecular Orbitals

Follow Aufbau sequence.



Step 3: Calculate Bond Order

$N_b = 10, N_a = 6$.
B.O. = $\frac{1}{2}(10 - 6) = 2$ (Double Bond).

Step 4: Diagnose Magnetism

Two unpaired electrons in the π^* antibonding orbitals =
Paramagnetic.

Revision Frame: MO Predictive Rules

Stability & Bond Order

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

- $N_b > N_a$ = Stable ↑
- $N_b \leq N_a$ = Unstable ↓

Bond Nature

- B.O. 1 = Single Bond —
- B.O. 2 = Double Bond ==
- B.O. 3 = Triple Bond ≡

Bond Length

$$Length \propto \frac{1}{Bond\ Order}$$

↑ B.O. → ↓ Length

Magnetic Nature

- [↑↓] All Paired = Diamagnetic (Repelled) 
- [↑] Any Unpaired = Paramagnetic (Attracted) 



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