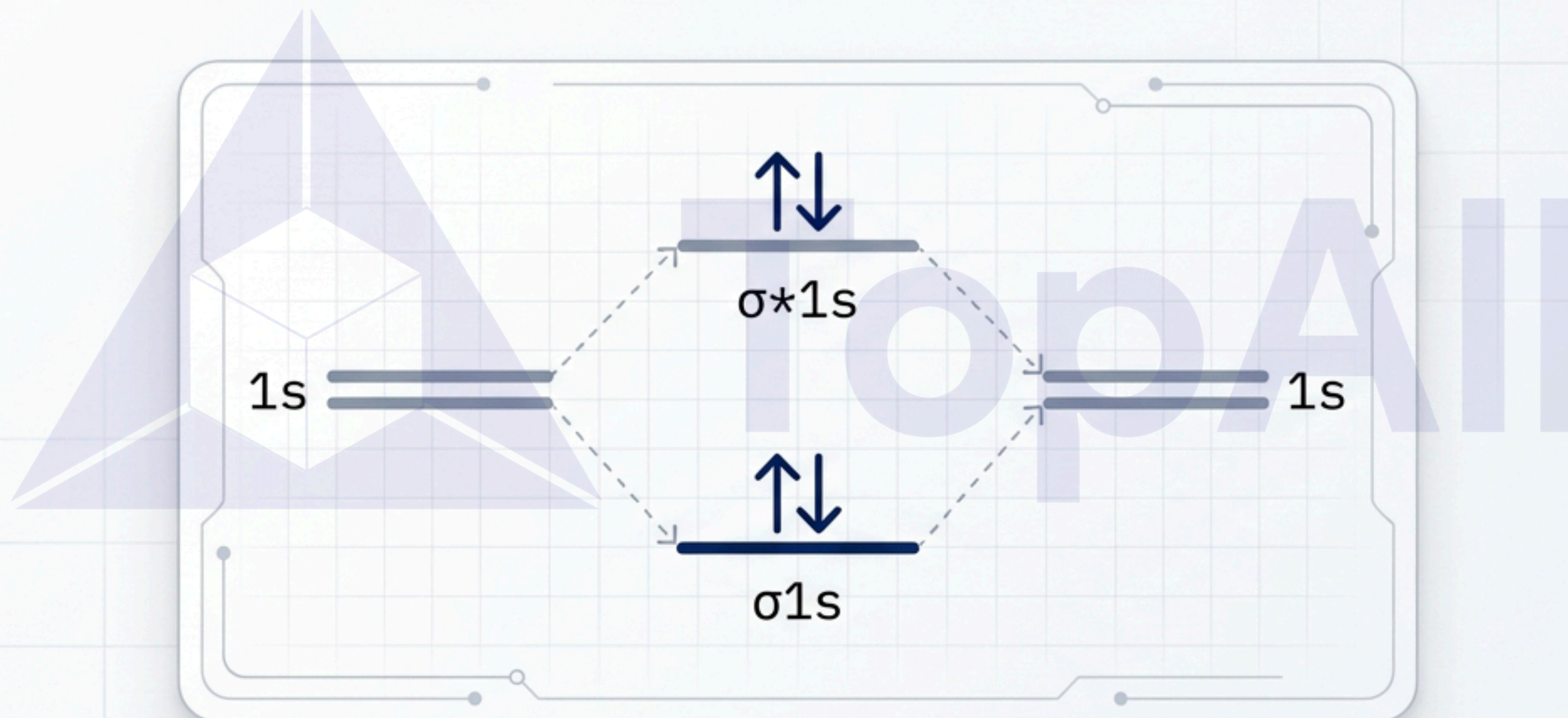


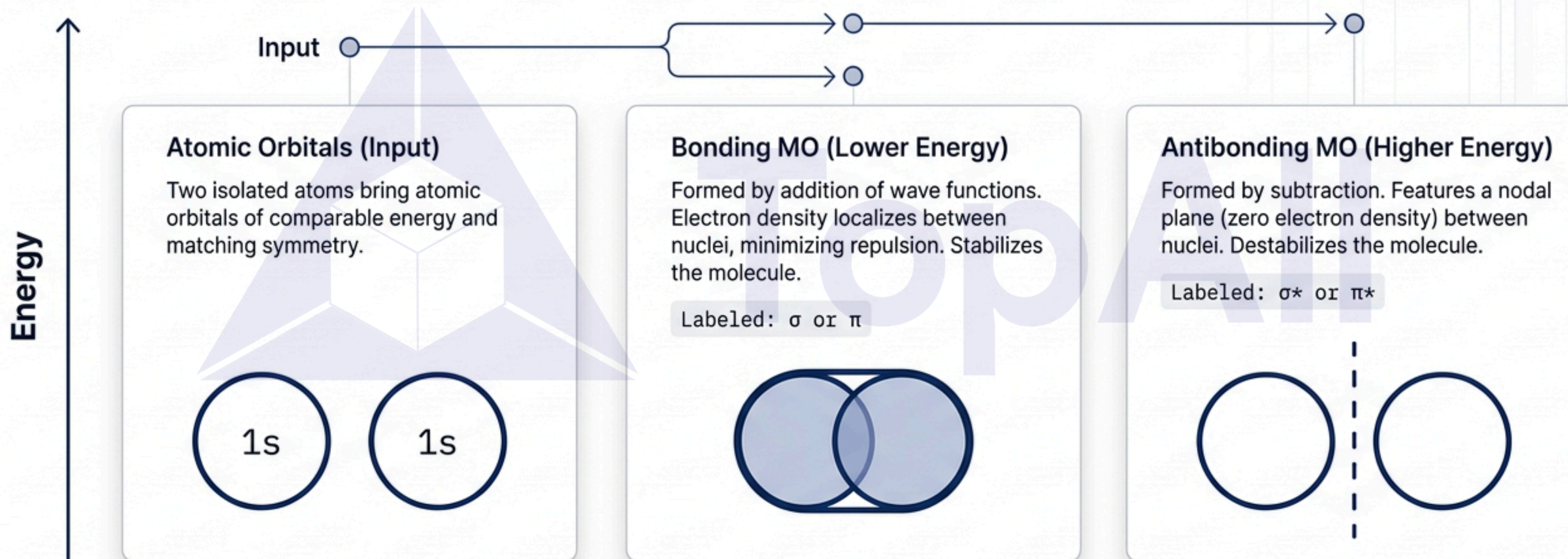
4.7.4 Energy Level Diagram for Molecular Orbitals

Predicting molecular stability, bond order, and magnetic behavior through electron population.



Constructing The Molecular Blueprint

Molecular orbitals are formed by the Linear Combination of Atomic Orbitals (LCAO). When two atomic orbitals combine, they conserve the total number of orbitals by splitting into two distinct energy states.



Conservation Rule: 2 Atomic Orbitals Combined = 1 Bonding MO + 1 Antibonding MO

The Two Pathways For Orbital Filling

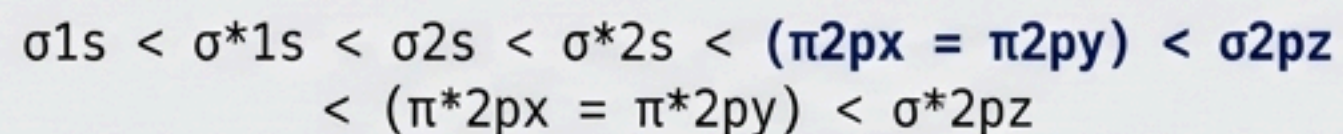
Electrons fill molecular orbitals following the Aufbau Principle, Pauli Exclusion Principle, and Hund's Rule. However, the exact energy sequence shifts based on the specific elements involved.

Exam Insight Pill

Always count total electrons first to choose the correct sequence pathway!

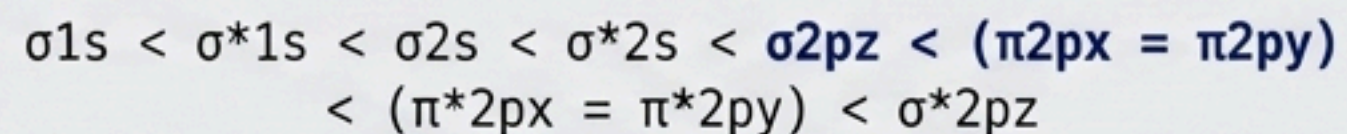
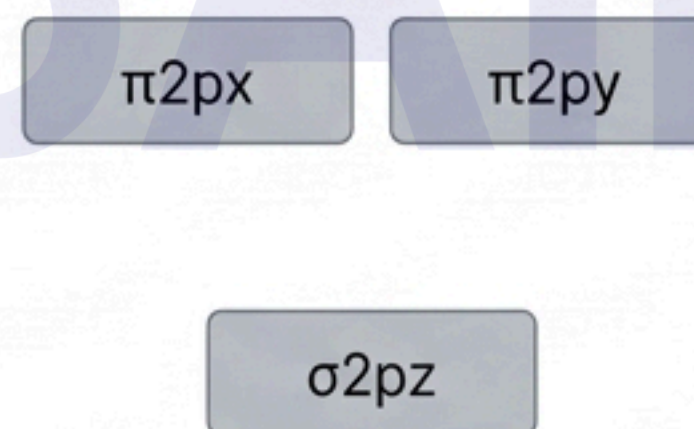
B_2 , C_2 , N_2 (Up to 14 electrons)

Rule Shift: The energy of the $\sigma 2p_z$ orbital is pushed higher than the $\pi 2p_x$ & $\pi 2p_y$ orbitals due to 2s-2p mixing.



O_2 and F_2 (More than 14 electrons)

Standard Rule: Normal energy sequence. The $\sigma 2p_z$ orbital is lower in energy than the π orbitals.





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Evaluating Molecular Stability

The distribution of electrons determines if a molecule can physically exist. We compare the number of electrons in bonding orbitals (N_b) against those in antibonding orbitals (N_a).

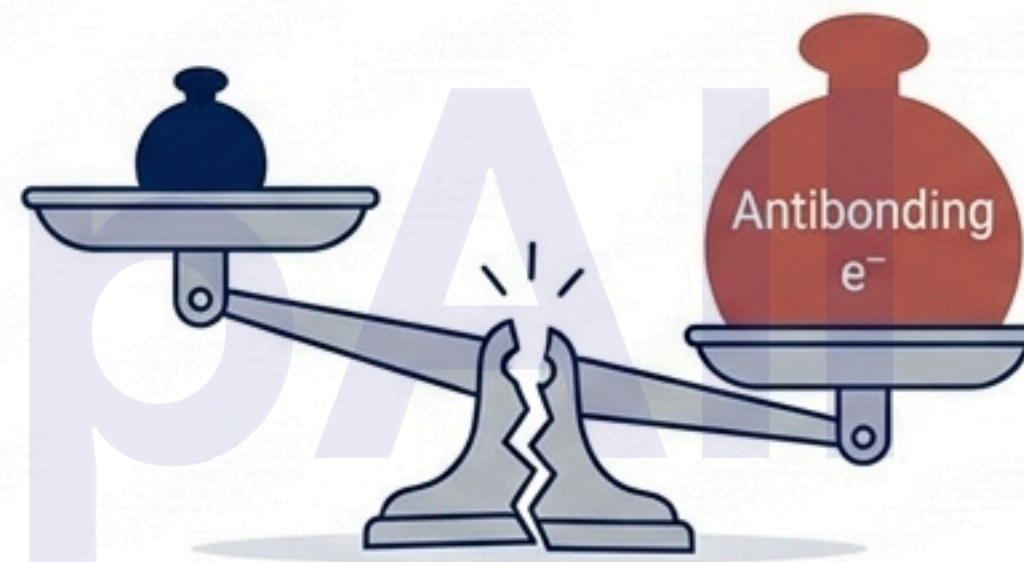
Bonding Dominance ($N_b > N_a$)



More electrons sit in stabilizing lower-energy orbitals. The bonding influence successfully overcomes nuclear repulsion.

Stable Molecule (e.g., Li_2)

Antibonding Dominance/Equality ($N_b \leq N_a$)



Antibonding influence equals or exceeds bonding. The electrons destabilize the nuclei.

Unstable Molecule (Does not exist, e.g., He_2 or Be_2)

Nature favors minimum energy. Placing electrons in antibonding orbitals actively cancels the energetic benefits of bonding.

Calculating Bond Order (B.O.)

Bond order acts as a mathematical proxy for bond strength, length, and multiplicity (single, double, triple bonds).

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

Where N_b = Bonding electrons, N_a = Antibonding electrons

1, 2, or 3

Corresponds exactly to single, double, or triple covalent bonds (e.g., O_2 has B.O. = 2).

≤ 0

Molecule cannot exist (e.g., Be_2 has B.O. = 0).

0.5, 1.5...

Fractional B.O. indicates resonance or odd-electron species (e.g., O_2^-).

As Bond Order Increases → Bond Enthalpy Increases & Bond Length Decreases

FIG. 4.21 SYNTHESIS

Period 2 Molecular Dashboard

Molecule	Valence e ⁻ Config	Bond Order	Magnetic Nature
B ₂	$(\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^1 (\pi 2p_y)^1$	1	Paramagnetic
C ₂	$(\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^2 (\pi 2p_y)^2$	2	Diamagnetic
N ₂	$(\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^2 (\pi 2p_y)^2 (\sigma 2p_z)^2$	3	Diamagnetic
O ₂	$\dots (\sigma 2p_z)^2 (\pi 2p_x)^2 (\pi 2p_y)^2 (\pi^* 2p_x)^1 (\pi^* 2p_y)^1$	2	Paramagnetic
F ₂	$\dots (\pi^* 2p_x)^2 (\pi^* 2p_y)^2$	1	Diamagnetic

Key-Takeaway Panel

Notice C₂ features a double bond made entirely of π bonds (no $\sigma 2p_z$ electrons), and O₂ has a double bond but is uniquely paramagnetic due to two unpaired π^* electrons.

Energy Diagrams Predict Reality

Molecular Orbital energy diagrams are not just abstract drawings; they successfully predict the **physical and chemical realities** of molecules that classical Lewis structures cannot explain.



1. Predicts Existence

If $N_b > N_a$ (Bond Order > 0), the molecule can physically exist in reality.



2. Predicts Strength & Length

Direct correlation: Higher Bond Order yields shorter, stronger molecular bonds.



3. Predicts Magnetism

Diamagnetic: All MOs doubly occupied (repelled by magnetic field)

Paramagnetic: Contains unpaired electrons (attracted by magnetic field)

Exam-Smart: The Ultimate Proof: Lewis theory suggests O_2 has all paired electrons. MO Theory correctly predicts O_2 is paramagnetic because of two unpaired electrons in its π^* antibonding orbitals.



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