Is it paramagenetic (A) or diamagnetic (B)?

\[ \text{N}_2 \]

\|
A & B & C & D & E & F & G \\
0 & .5 & 1 & 1.5 & 2 & 2.5 & 3 \\

\[ \text{O}_2 \]

\[ \text{O}_2 \]

\[ \text{Li} \quad \text{Be} \quad \text{B} \quad \text{C} \quad \text{N} \quad \text{O} \quad \text{F} \]

Splitting between s and p is greater as atomic charge increases.

This means less s and p interaction.

\[ \text{Atomic Orbital Energies} \]

<table>
<thead>
<tr>
<th></th>
<th>H</th>
<th>Li</th>
<th>Be</th>
<th>B</th>
<th>C</th>
<th>N</th>
<th>O</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-1313</td>
<td>-6505</td>
<td>-20204</td>
<td>-29735</td>
<td>-41034</td>
<td>-54265</td>
<td>-69268</td>
<td></td>
</tr>
<tr>
<td>2s</td>
<td>-515</td>
<td>-1299</td>
<td>-1853</td>
<td>-2482</td>
<td>-3267</td>
<td>-4129</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2p</td>
<td>-814</td>
<td>-1138</td>
<td>-1490</td>
<td>-1659</td>
<td>-1917</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2p - 2s</td>
<td>485</td>
<td>715</td>
<td>991</td>
<td>1608</td>
<td>2212</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The gap between 2p and 2s grows as you increase Z.
Liquid oxygen poured into the space between the poles of a strong magnet remains there until it boils away.

Attraction to a magnetic field shows that O\textsubscript{2} molecules have unpaired electrons.

Is it paramagenetic (A) or diamagnetic (B)?

<table>
<thead>
<tr>
<th>Energy</th>
<th>B.O.</th>
<th>Bond Length</th>
<th>Energy</th>
<th>B.O.</th>
<th>Bond Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>H\textsubscript{2}</td>
<td>1</td>
<td>0.74Å</td>
<td>H\textsubscript{2}\textsuperscript{+1}</td>
<td>0.5</td>
<td>1.06Å</td>
</tr>
<tr>
<td>H\textsubscript{2}\textsuperscript{+1}</td>
<td>0.5</td>
<td>1.08Å</td>
<td>O\textsubscript{2}\textsuperscript{+1}</td>
<td>2.5</td>
<td>1.12Å</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>2</td>
<td>1.21Å</td>
<td>O\textsubscript{2}\textsuperscript{-1}</td>
<td>1.5</td>
<td>1.28Å</td>
</tr>
<tr>
<td>O\textsubscript{2}\textsuperscript{-2}</td>
<td>1</td>
<td>1.49Å</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Orbitals are not symmetrical

\begin{align*}
\text{C} & \cdots \text{O} \\
\pi & \quad \pi^* \\
\text{C} & \cdots \text{O}
\end{align*}
Orbitals are not symmetrical

\[ \text{C--O} \quad \pi \quad \text{C--O} \quad \pi^* \]

Clicker Quiz

Draw a MO diagram for the molecule NO

What is the bond order?
A. 1  B. 1.5  C. 2  D. 2.5  E. 3

Which has the shortest bond distance?
A. NO⁺  B. NO  C. NO⁻

\[ \text{H–C≡C–H} \]

How can we construct the Molecular Orbitals for Acetylene?

Let us break the problem into parts.

Construct orbitals for \( \text{C}_2^2 \) and the add 2 H1s orbitals.

\( \text{C}_2^2 \) isoelectronic with \( \text{N}_2 \)

B.O. = 3

diamagnetic

\[ \text{H–C≡C–H} \]

Make two combinations of H 1s orbitals.
One + and one –
They are very far apart so their energy is the same.
Mainly $p$

average to give sp hybrids

Mainly $s$

$C_2^2$ $sp^2$ hybrids

Make two combinations of H 1s orbitals.
One + and one −
They are very far apart so their energy is the same.

$\sigma$ $\sigma^*$

$\sigma^*$ $\pi$ $\pi^*$

$\sigma^*$ $\sigma^*$ $\sigma^*$

From your textbook

sp hybrids

H s - C sp sigma bond

C sp - C sp sigma bond

Figure 14.4: The hybridization of the $s$, $p_x$, and $p_y$ atomic orbitals results in the formation of three $sp^2$ orbitals oriented in the $xy$ plane. The larger spheres of the orbitals lie in the plane, at angles of 120° to each other, and point toward the corners of a triangle.

$sp^3$ hybrids
\[ \Psi_1 = H_1 + H_2 + H_3 + H_4 \]

\[ \Psi_2 = H_1 + H_2 - H_3 - H_4 \]

\[ \Psi_3 = H_1 - H_2 + H_3 - H_4 \]

\[ \Psi_4 = H_1 - H_2 - H_3 + H_4 \]
C 2p + ψ₂

C 2s + ψ₁

H 1s LCAOs

ψ₁, ψ₂, ψ₃, ψ₄

2s

Individual H s orbitals

4 equal C sp³ - H s bonds

Delocalized Model

Hybrid Orbital Model

C

2p

sp³ hybrids

2s

4 equal C sp³ - H s bonds

3 bonds from C 2p
1 bond from C 2s

How many sp³ hybridized atoms?
How many sp² hybridized atoms?
How many sp² hybridized atoms?

N=\begin{array}{c}
\text{C} \\
\text{H₃N} \\
\text{CH₃}
\end{array}

How many sp³ hybridized atoms?
How many sp² hybridized atoms?
How many sp² hybridized atoms?