

# Molecular Orbital Theory

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YALE UNIVERSITY  
CHEMISTRY 161  
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## Reviewing Models of Chemical Structures

	<u>PROS</u>	<u>CONS</u>
<b>Lewis Structure:</b>	simple; good for $n = 1, 2$	2-dimensional only; all electrons paired; cannot predict magnetism; falters for: odd number electrons, resonance, multiple structures many exceptions ( $n \geq 3$ )
<b>VSEPR:</b>	expansion of Lewis; 3-dimensional; gives info on angles	all electrons paired; cannot predict magnetism;
<b>VALENCE BOND THEORY:</b>	gives geometric info; relatively simple	electrons localized to atoms; cannot predict magnetism easily

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*We need a model of chemical bonding that can capture this phenomenon!*

## VALENCE BOND vs. MOLECULAR ORBITAL

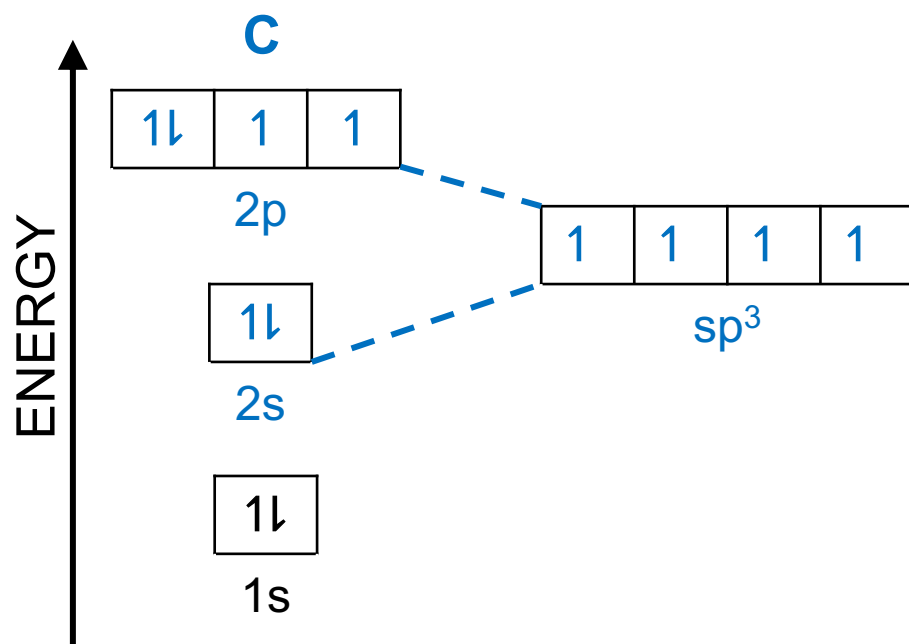
### *Valence Bond (VB) Theory*

Mixing atomic orbitals (AOs) within an atom.

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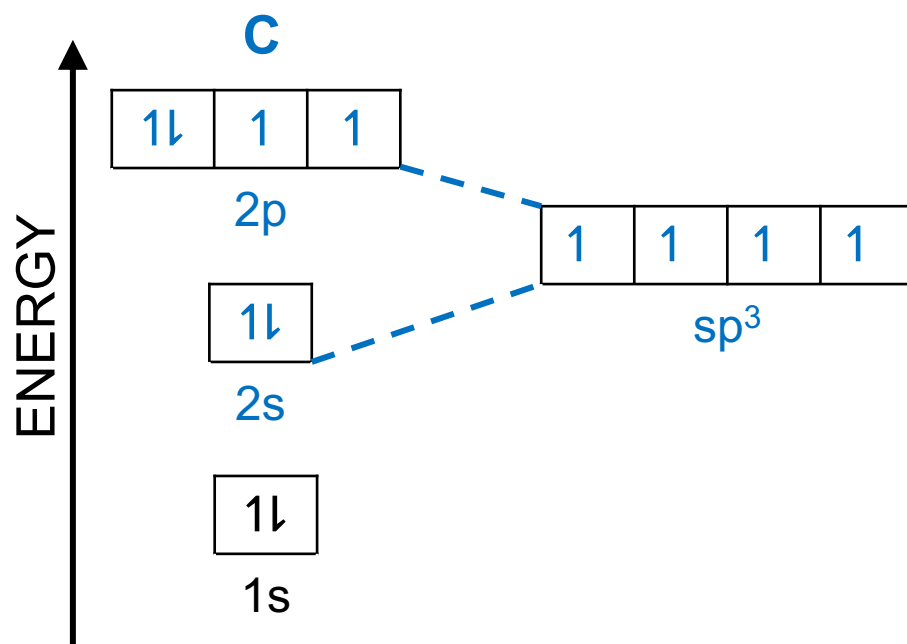


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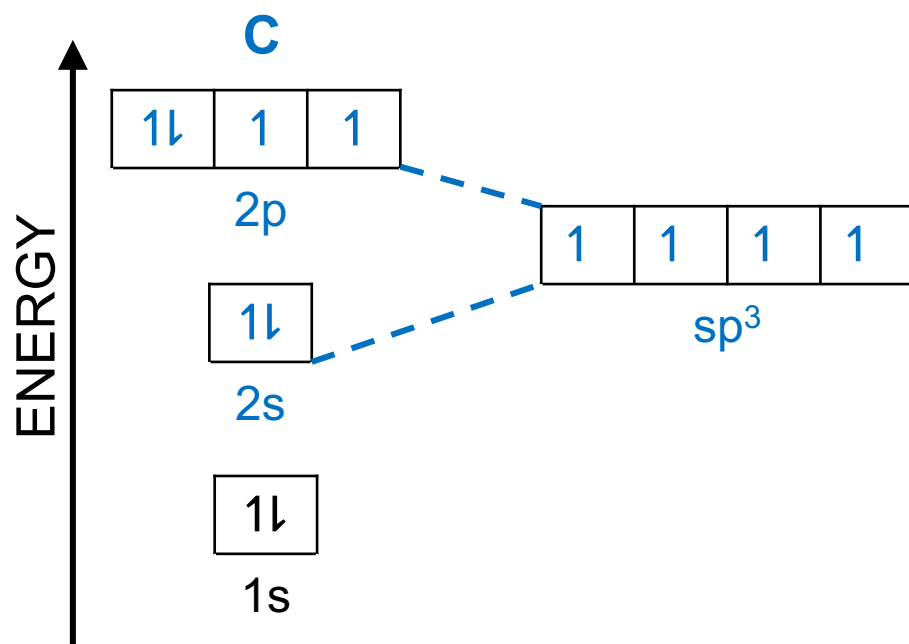
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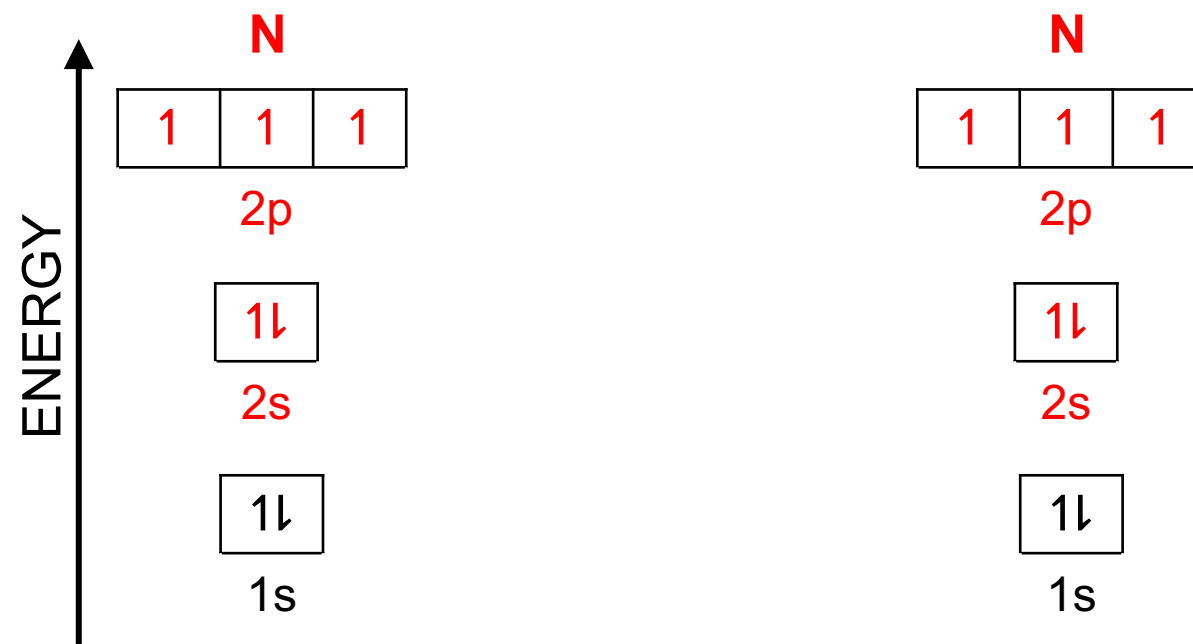


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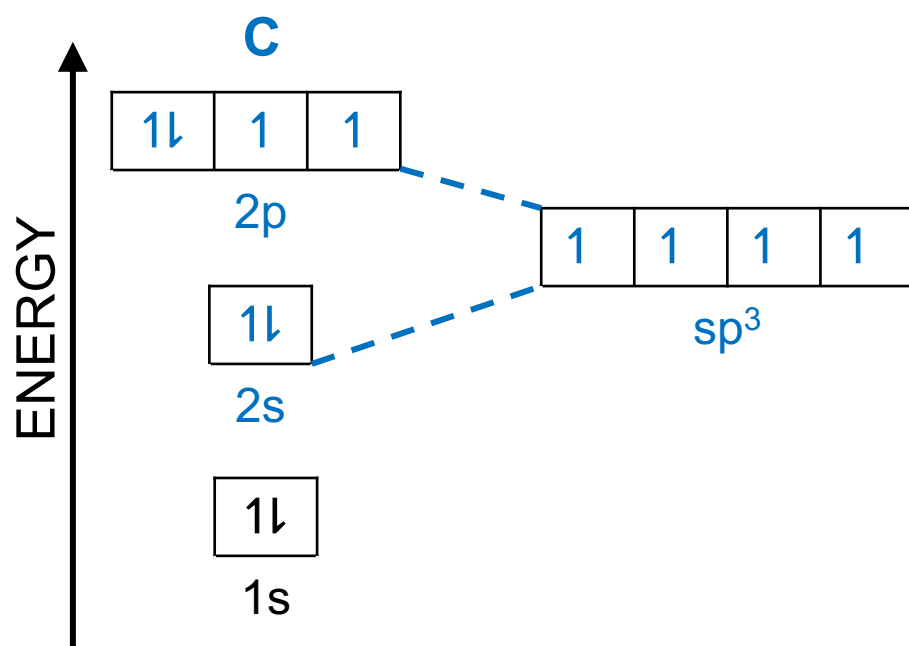
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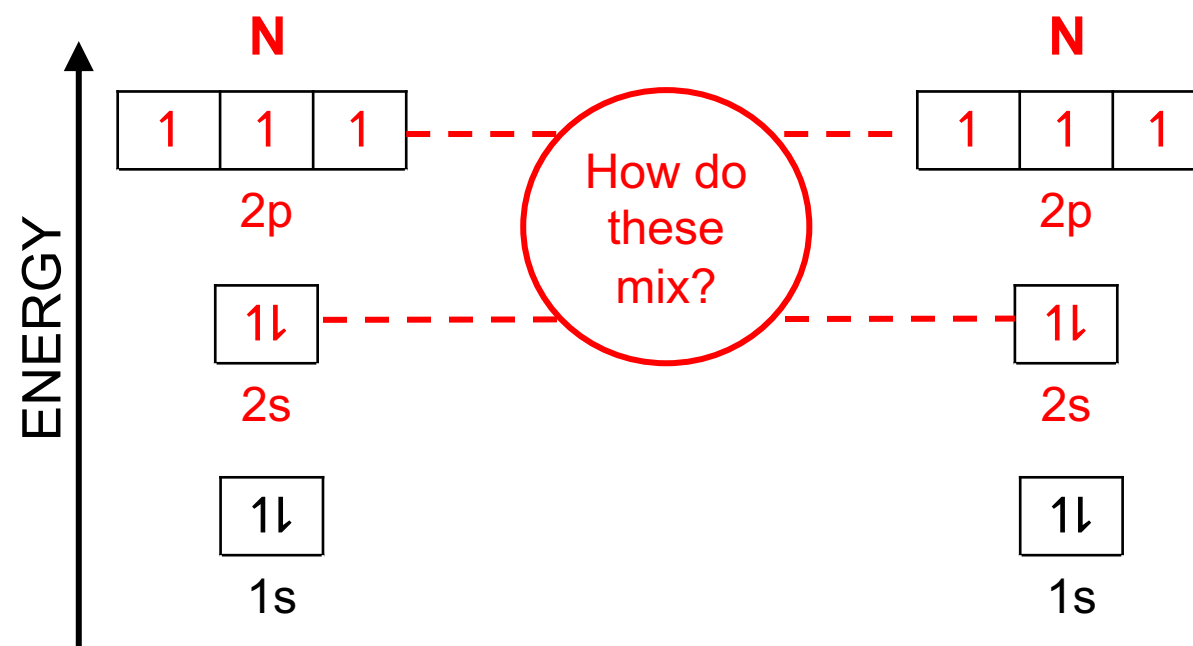


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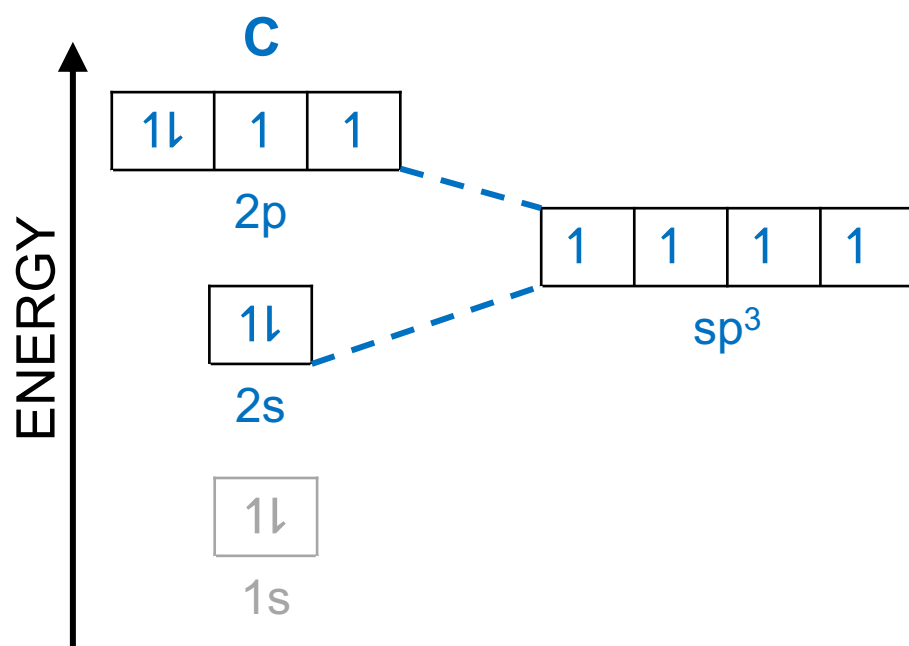
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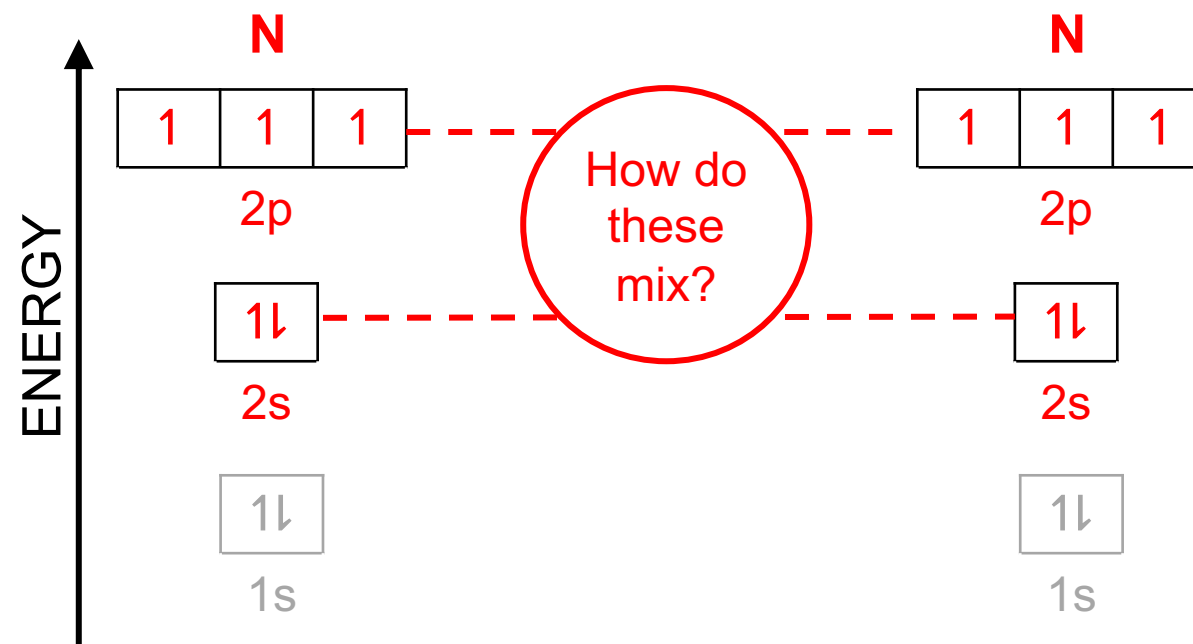
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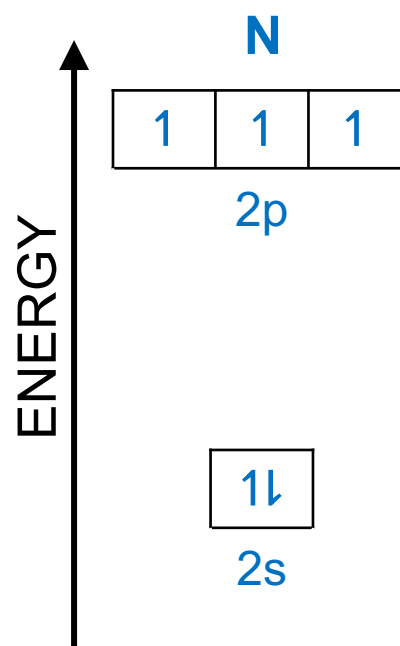
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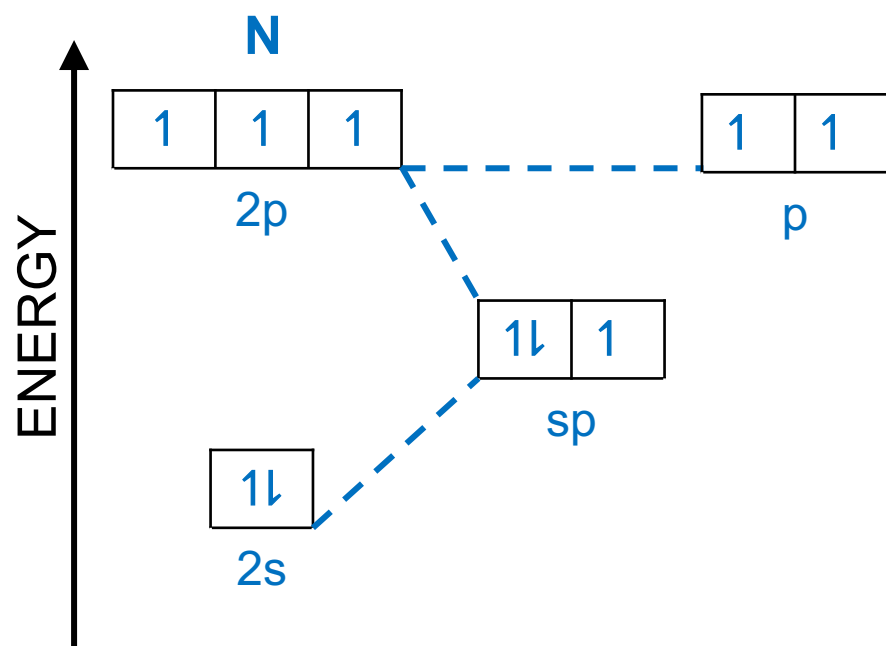
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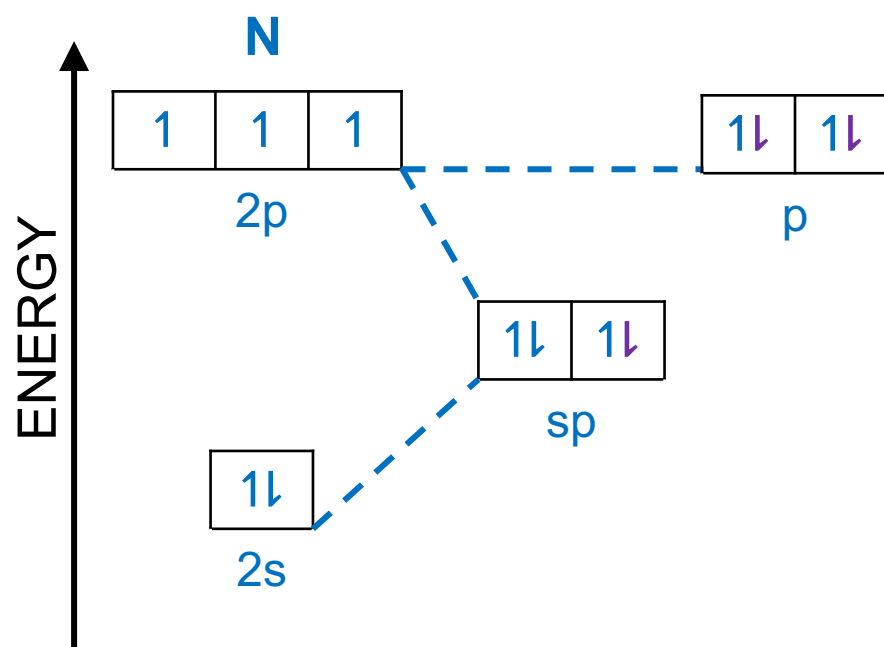
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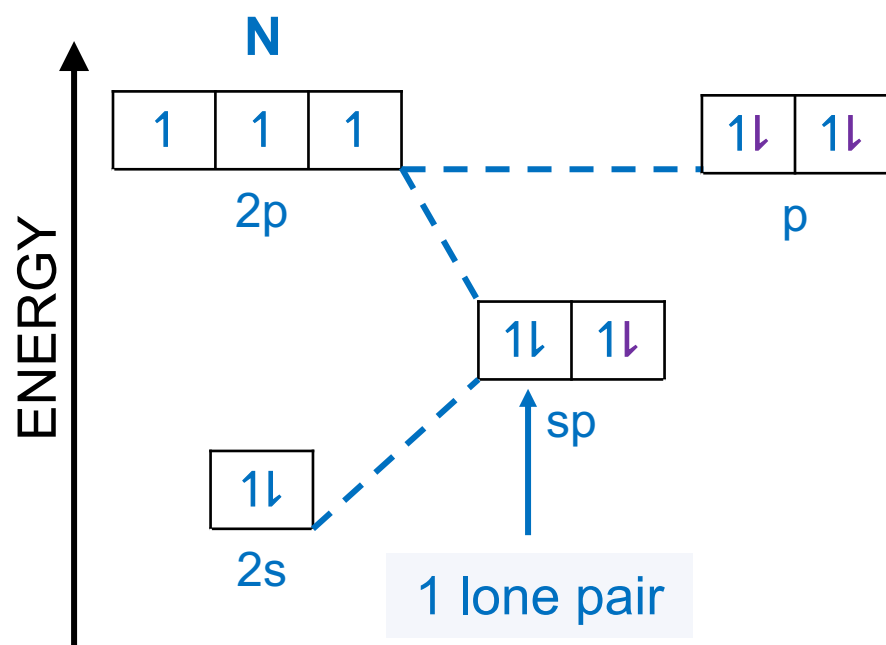
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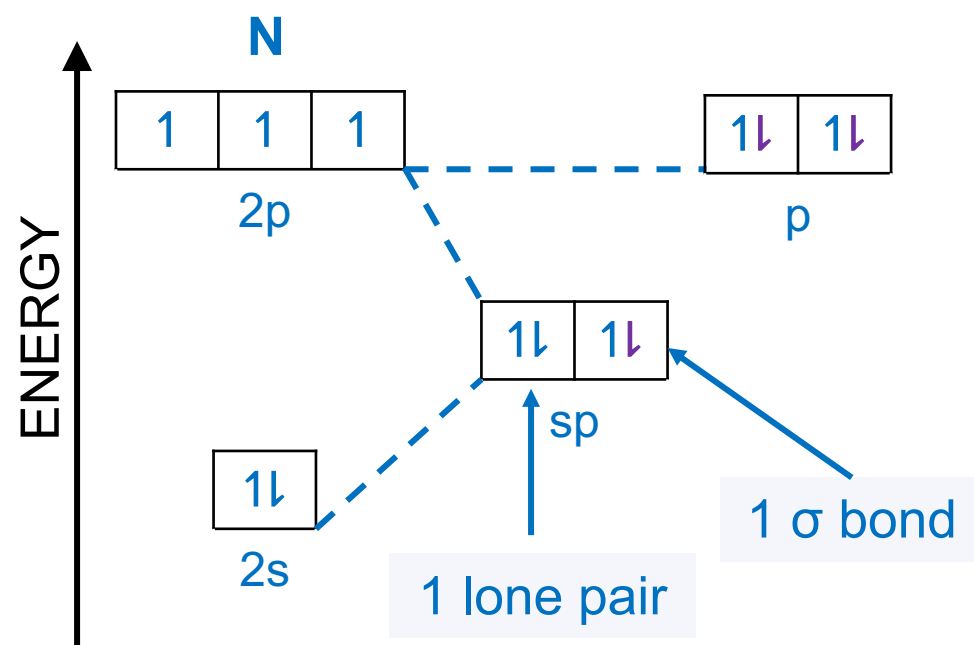
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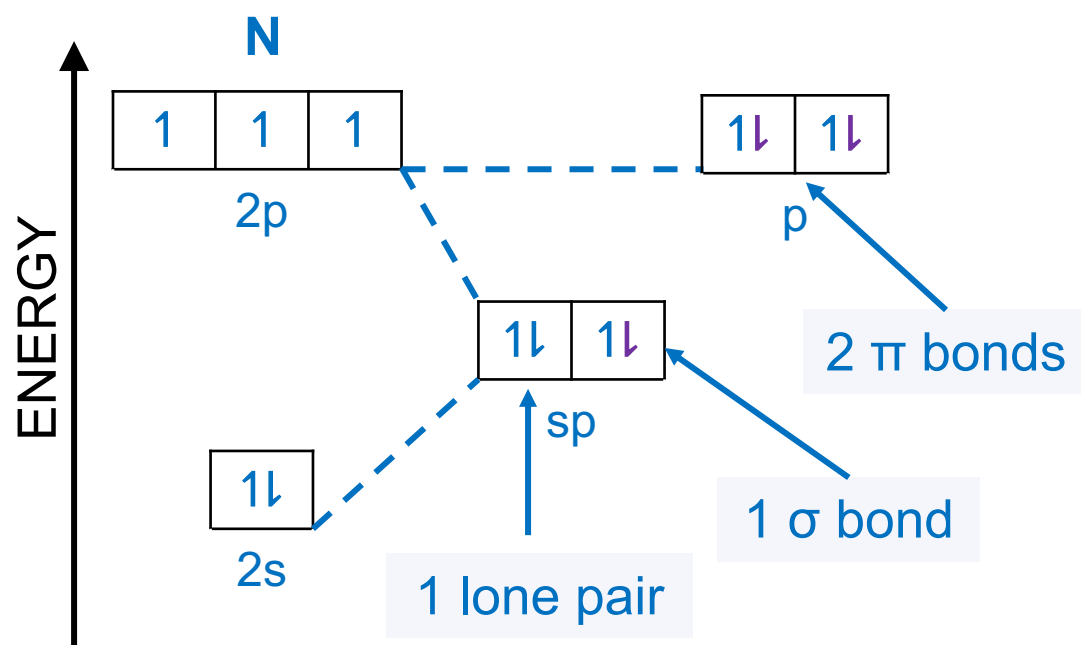
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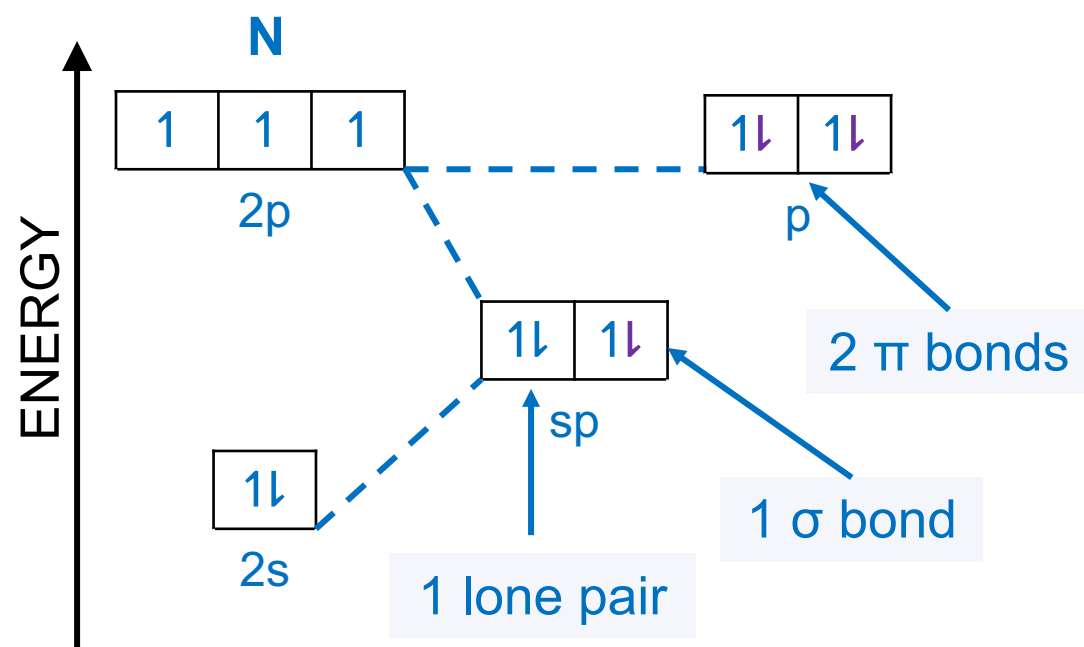
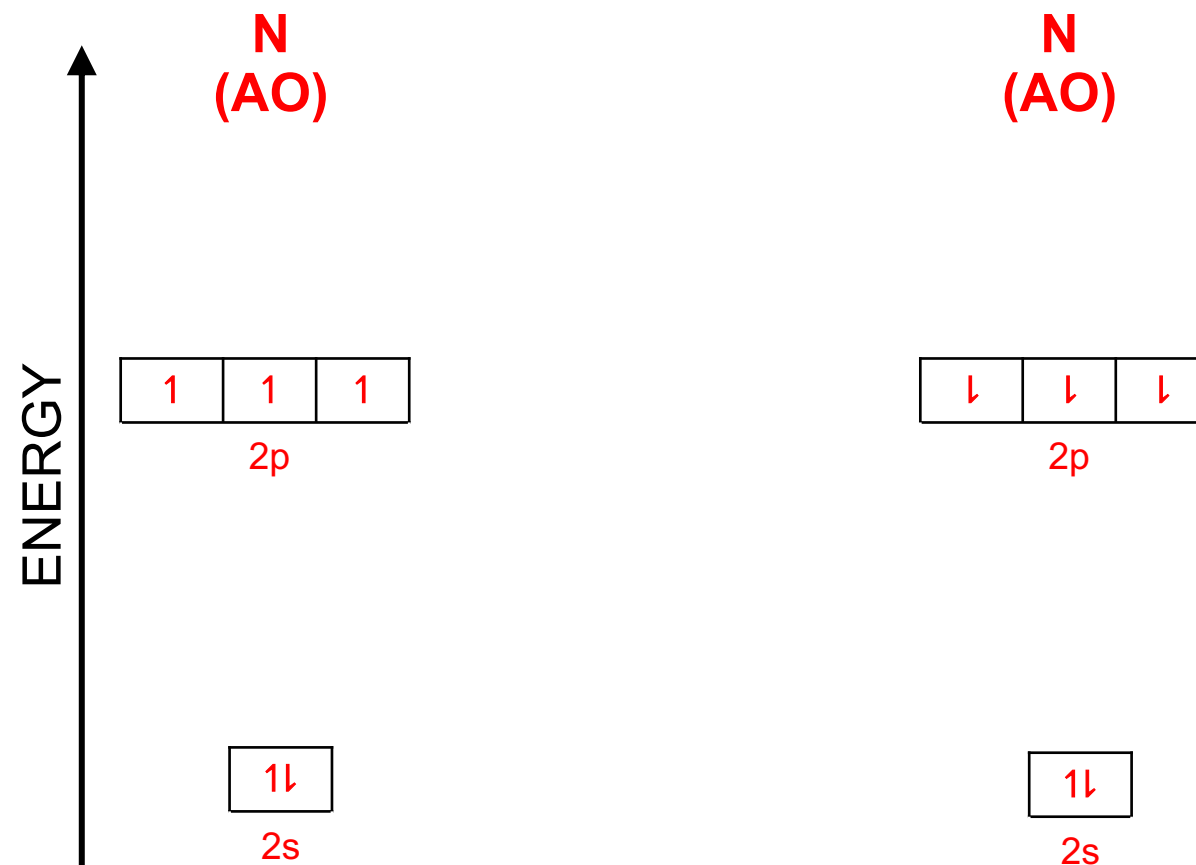
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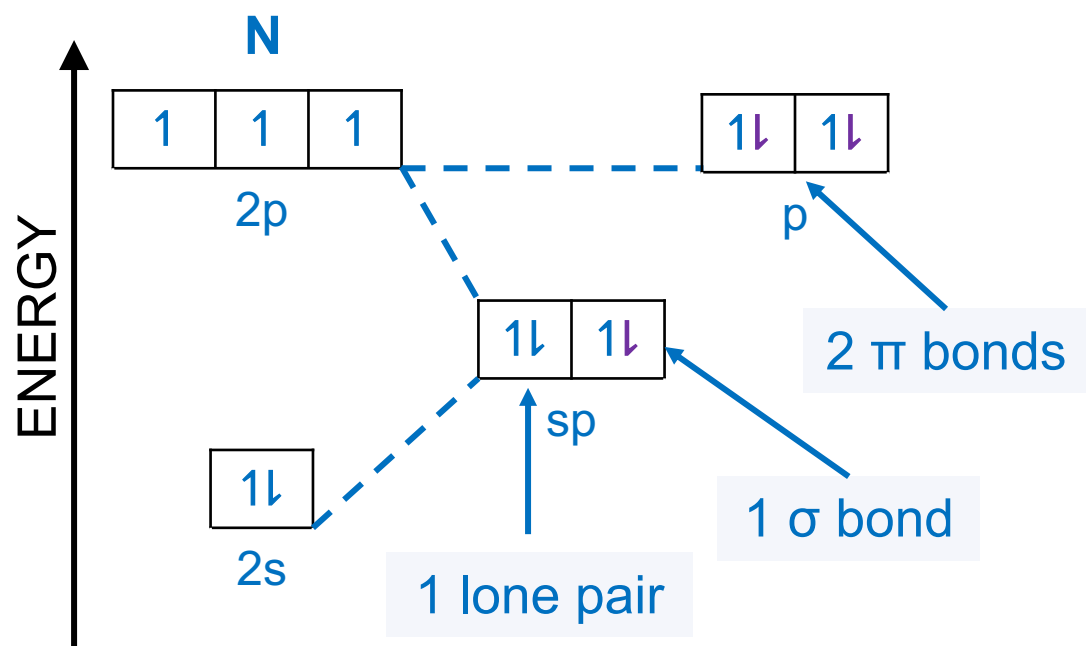
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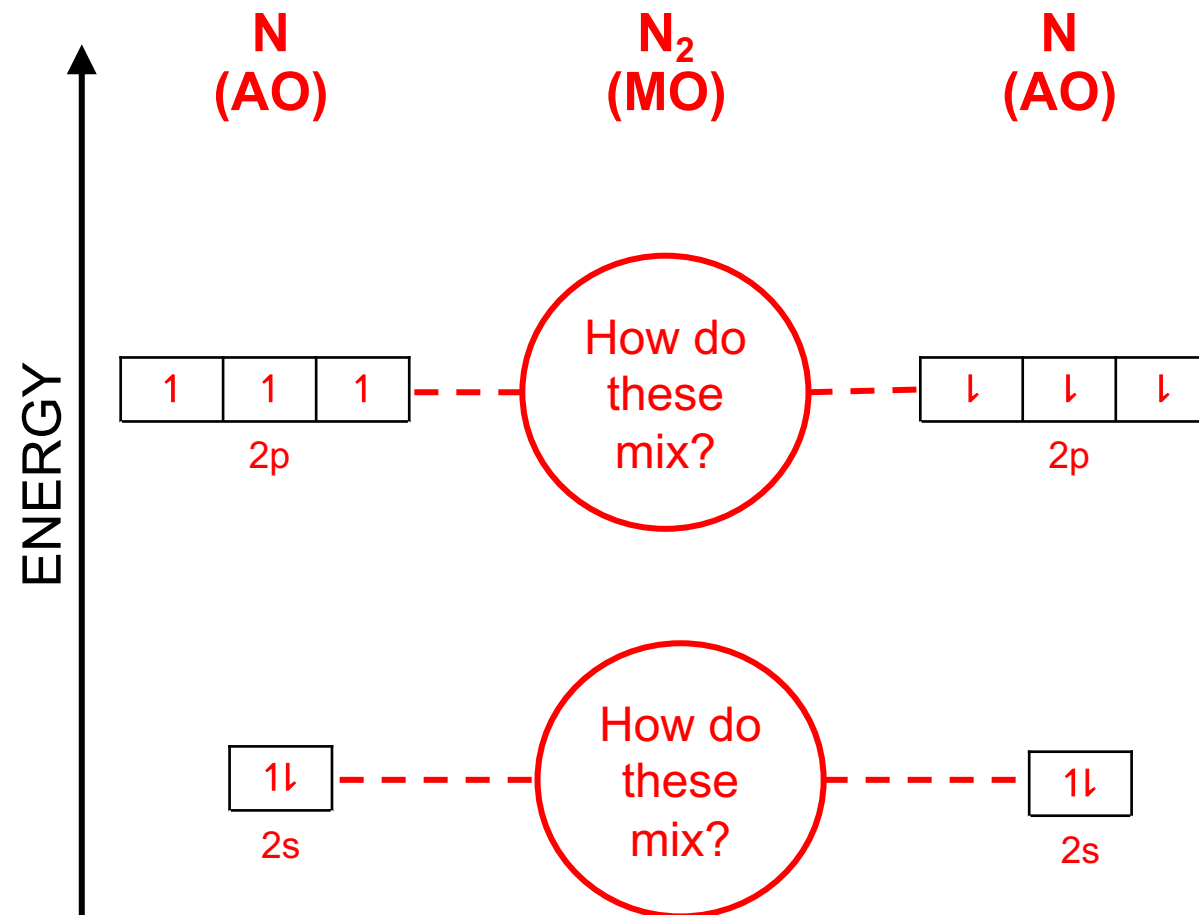
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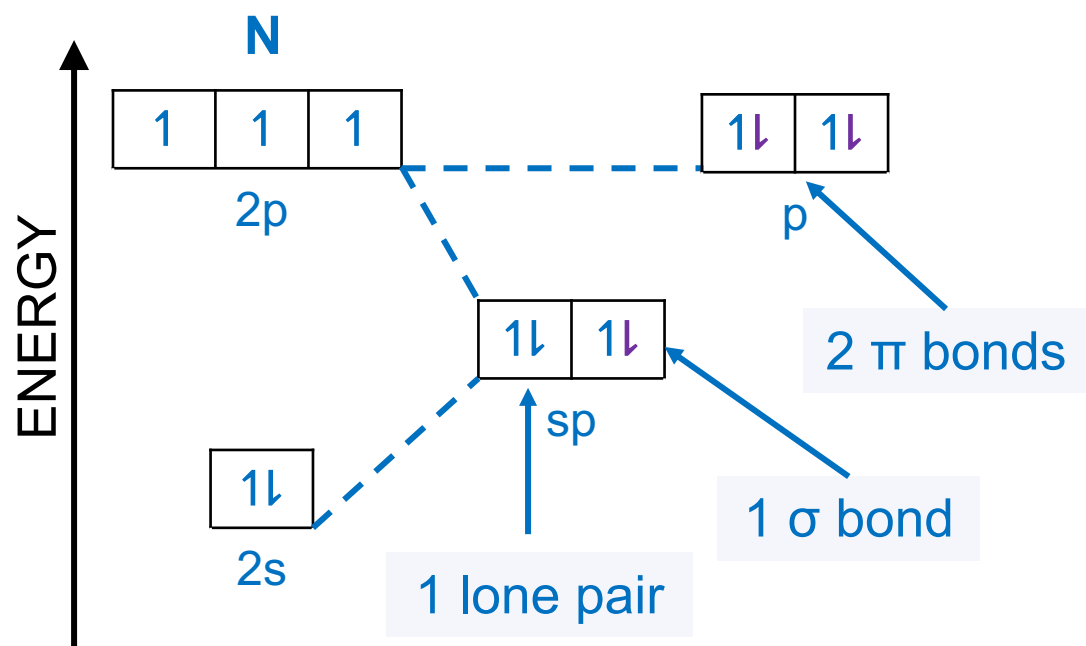
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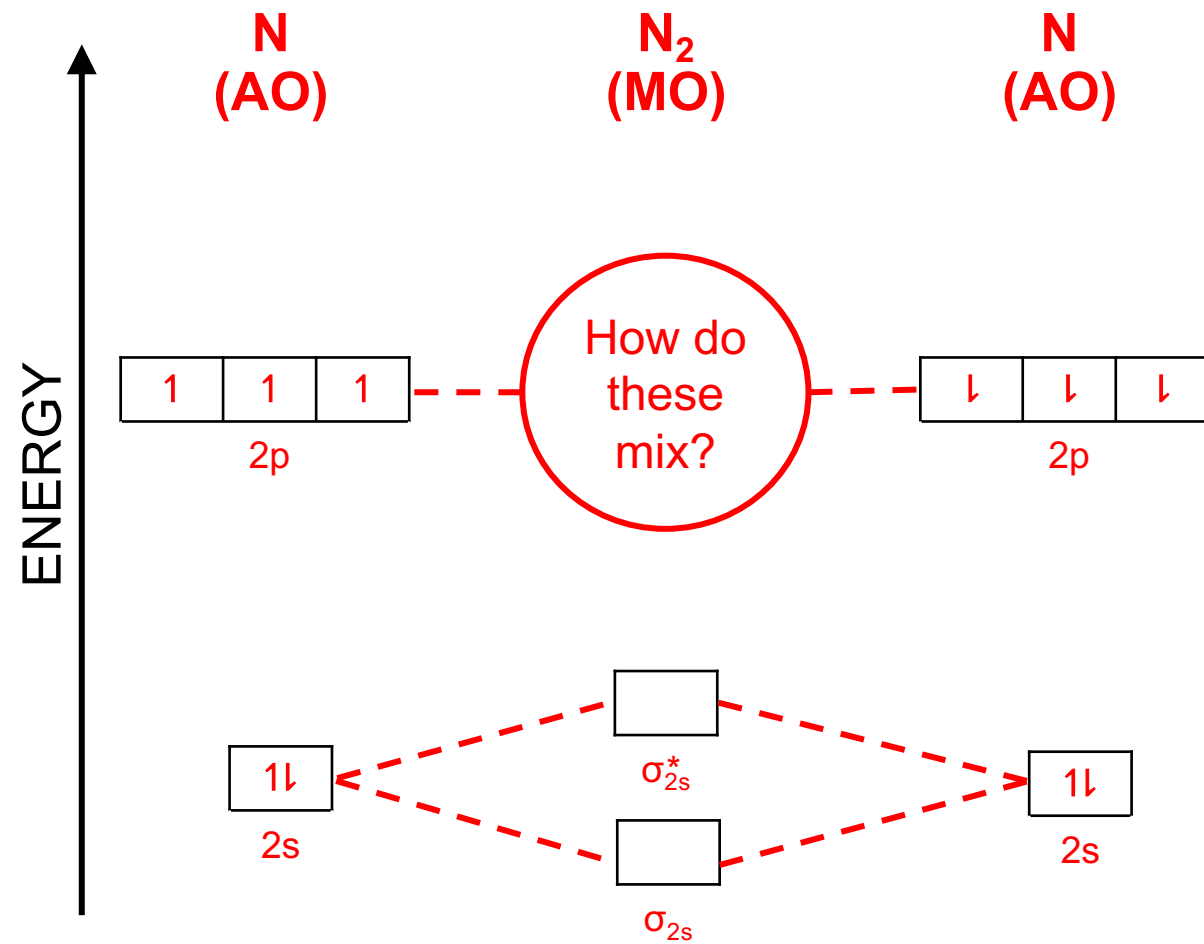
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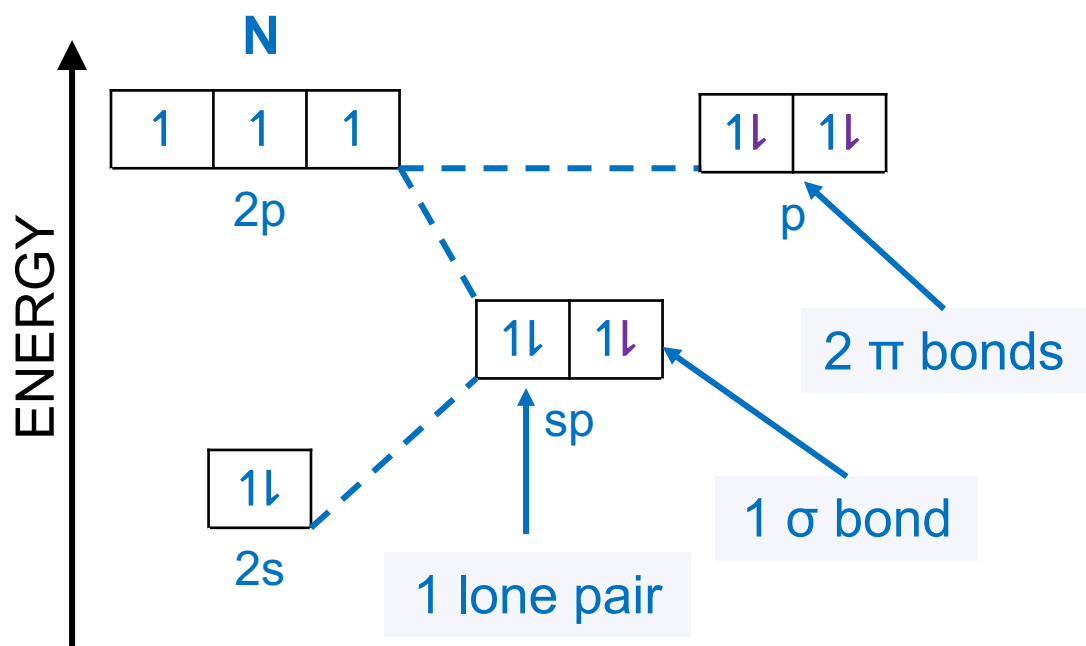
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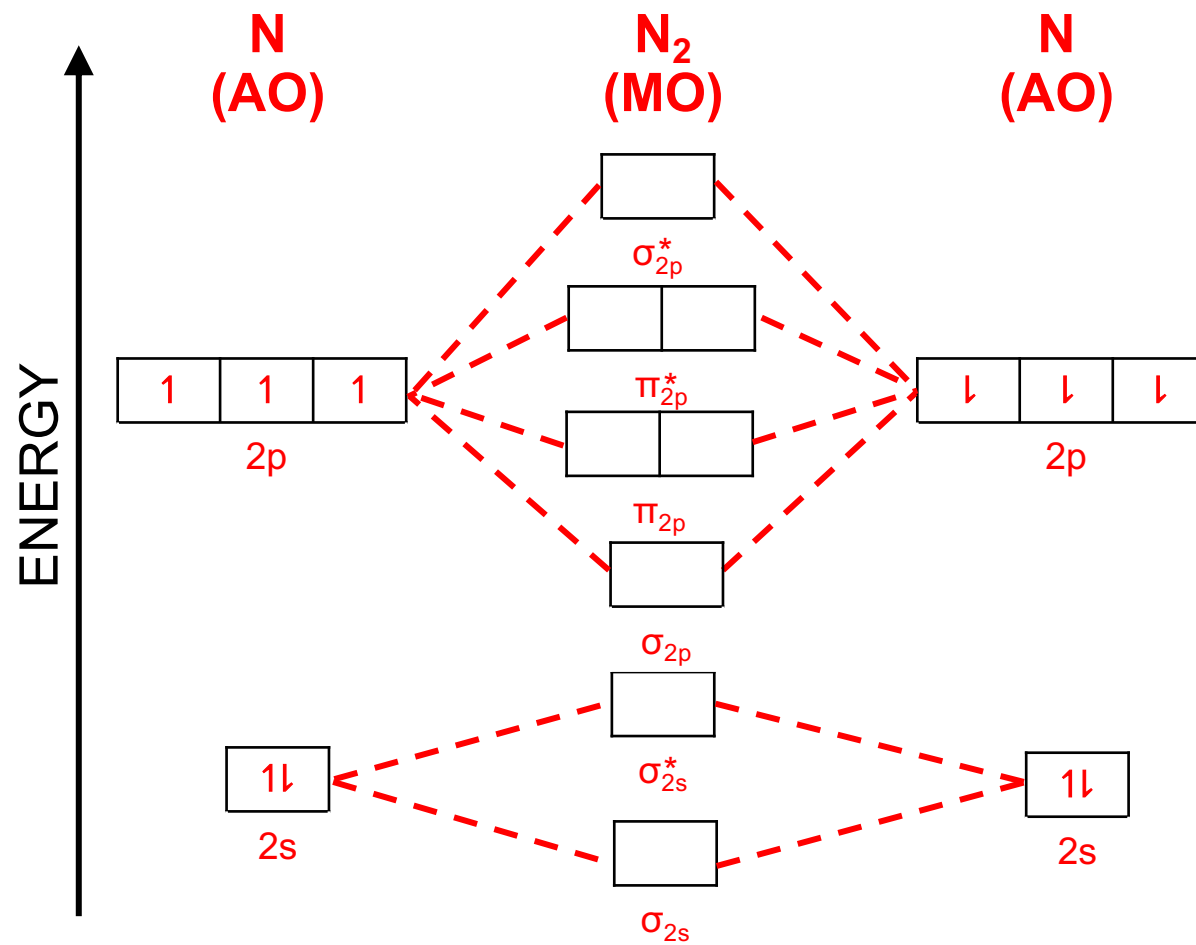
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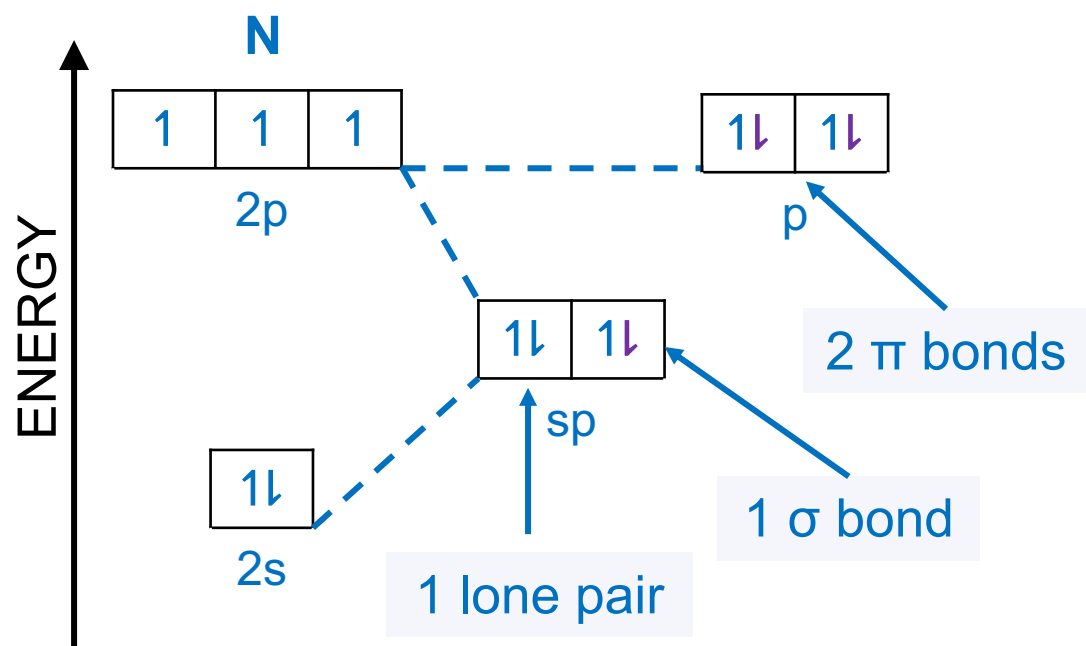
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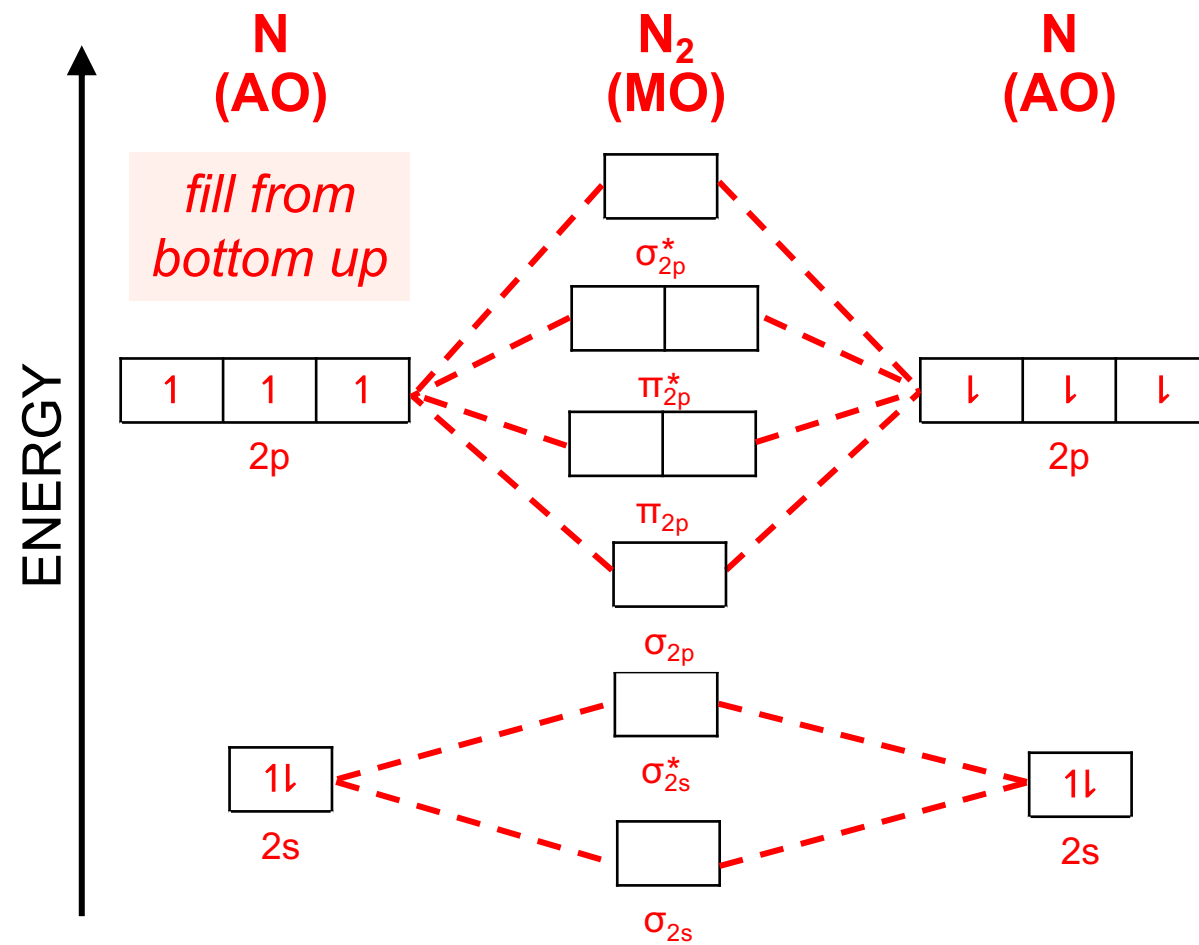
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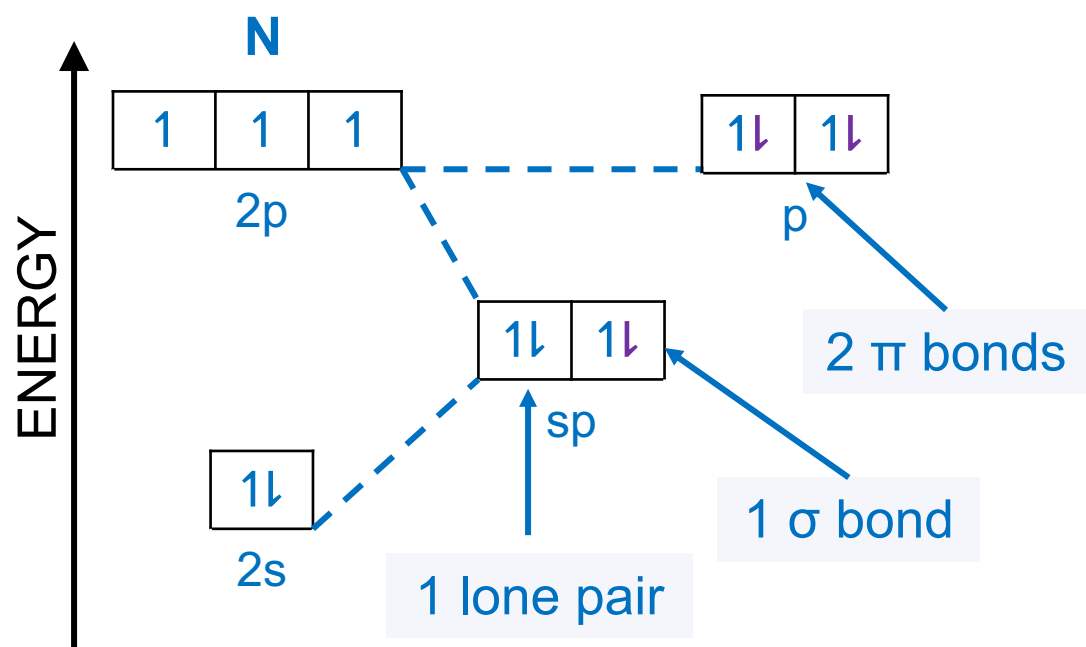
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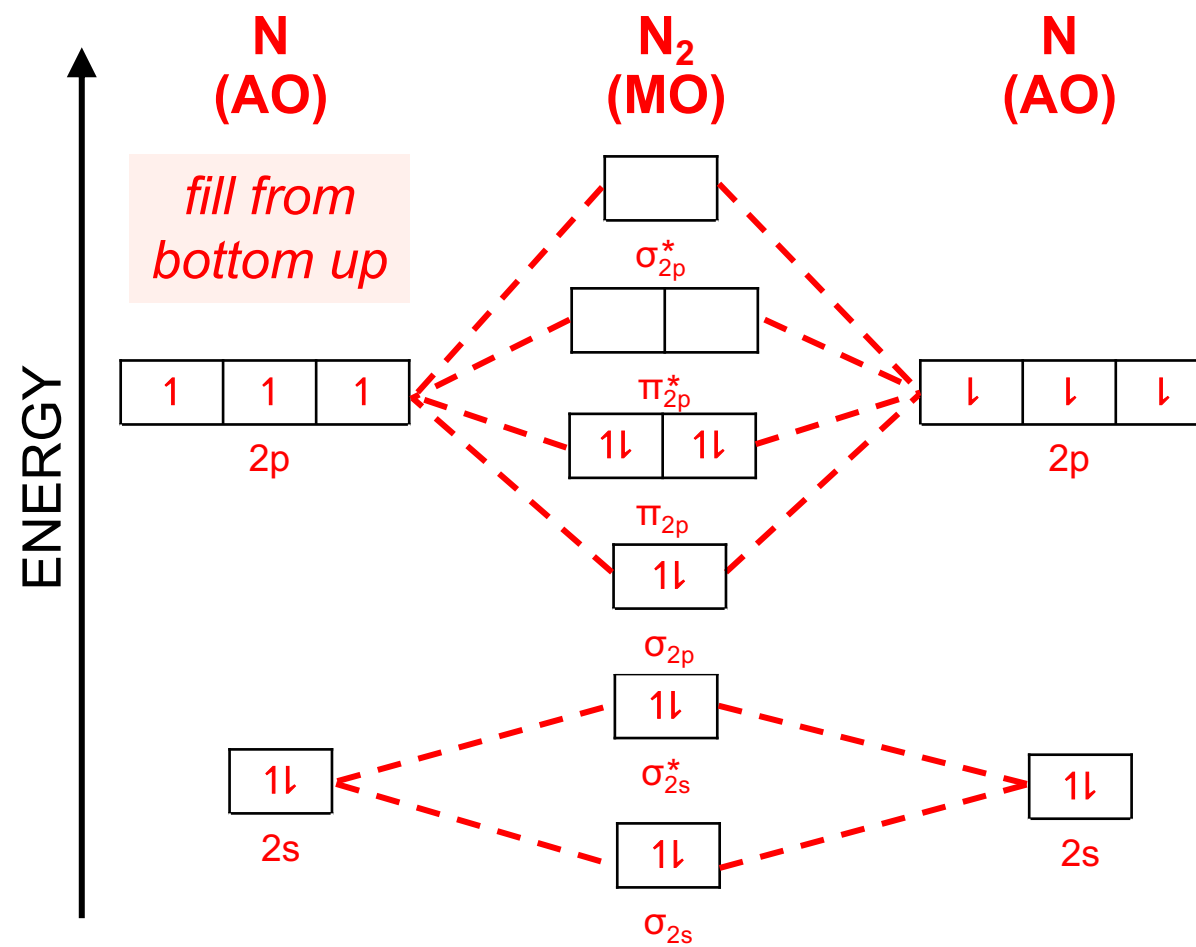


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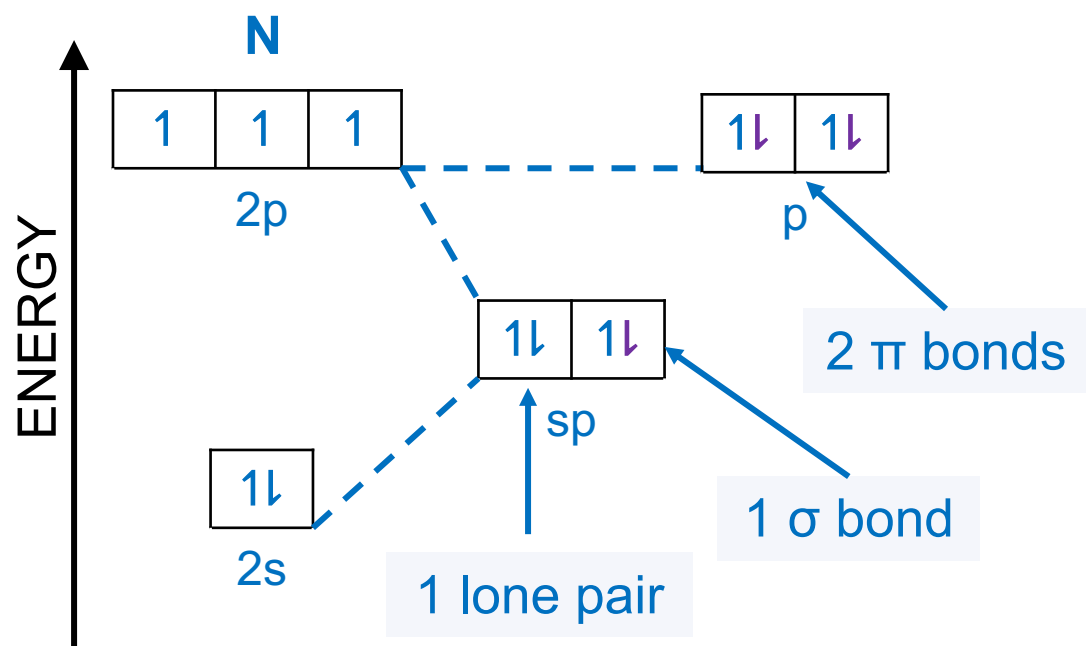
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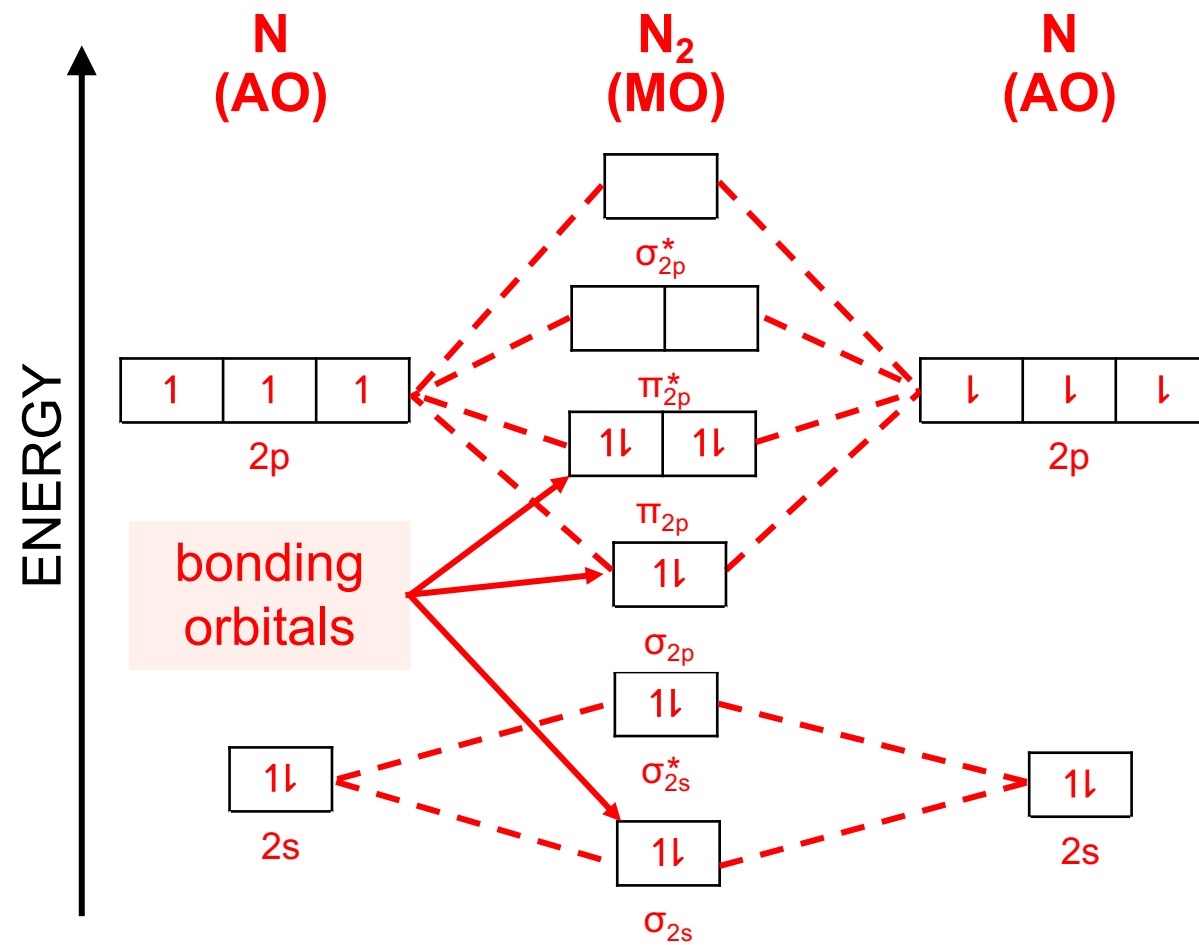
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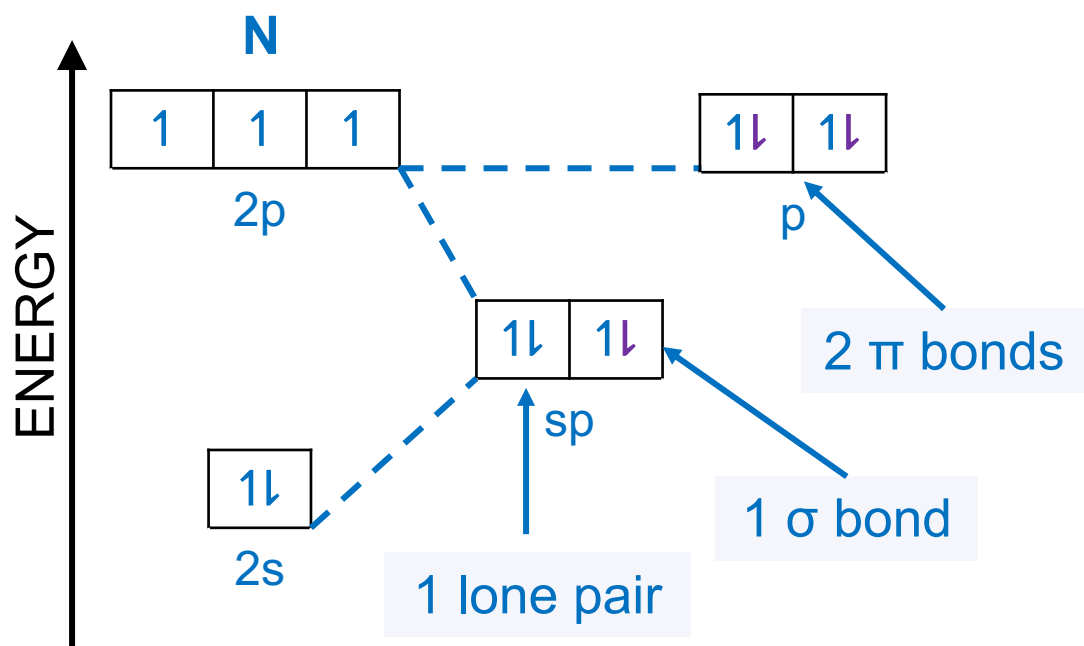
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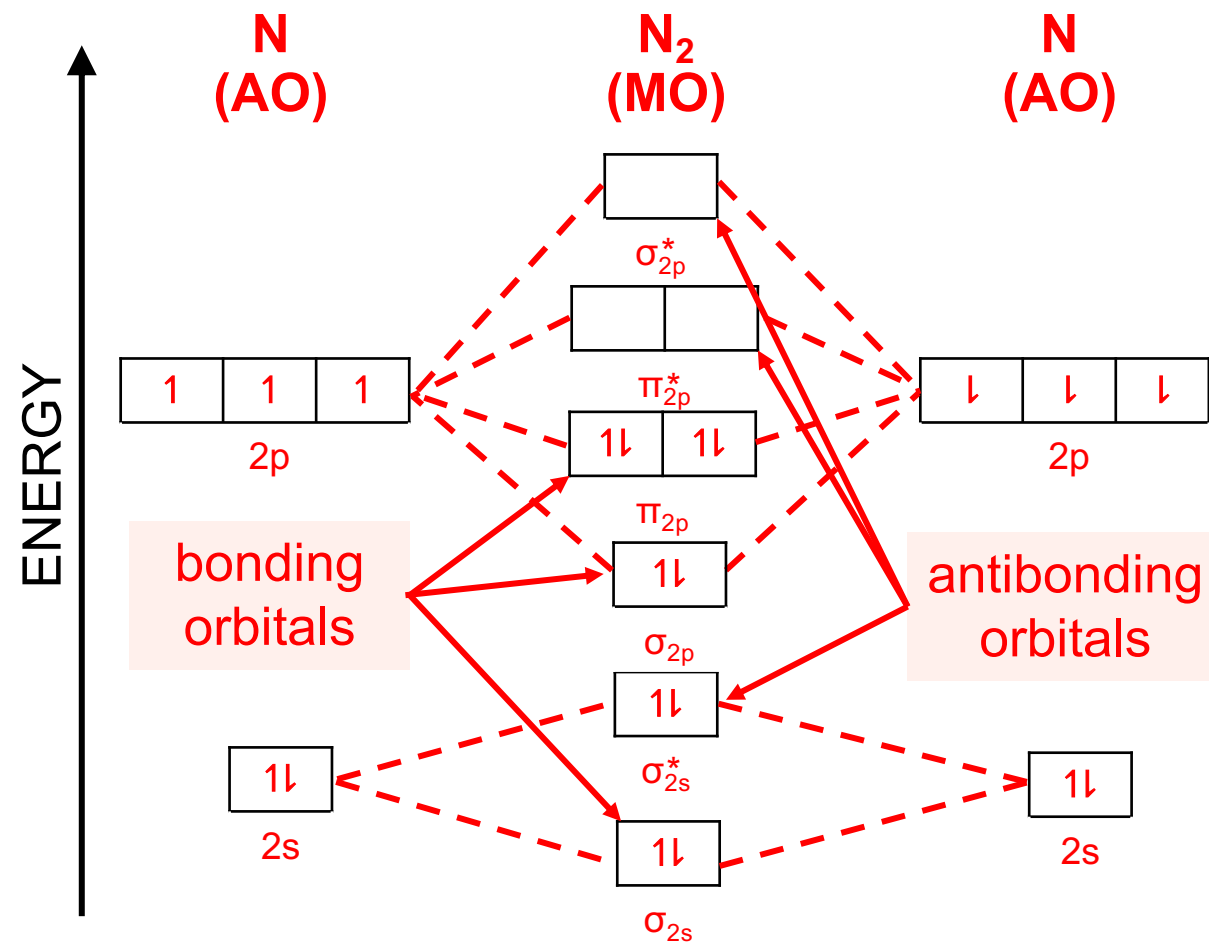
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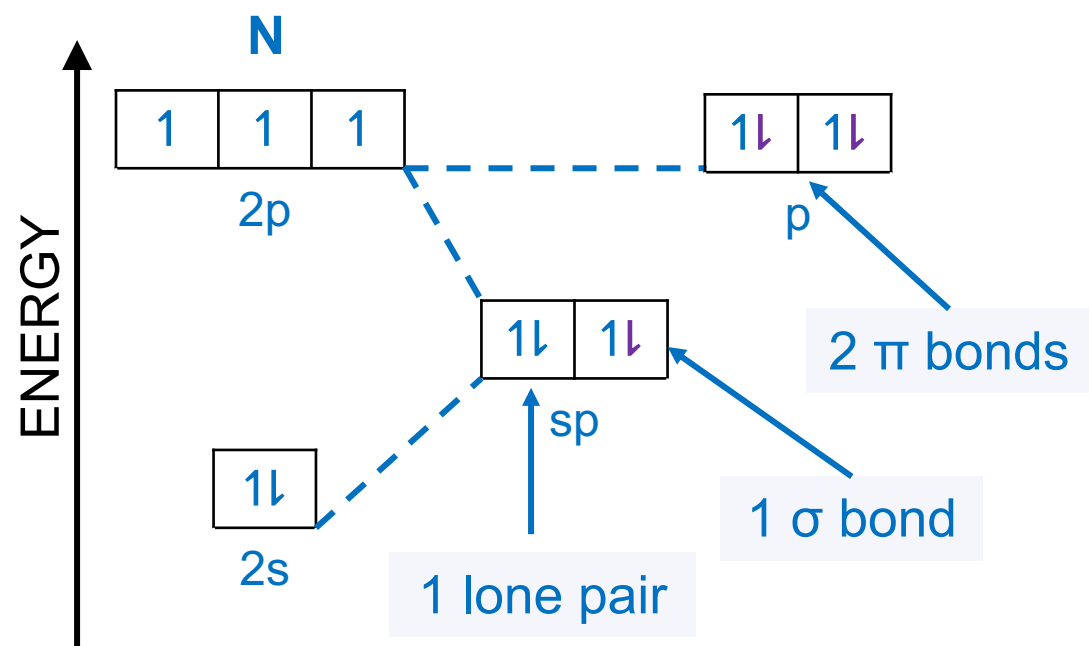


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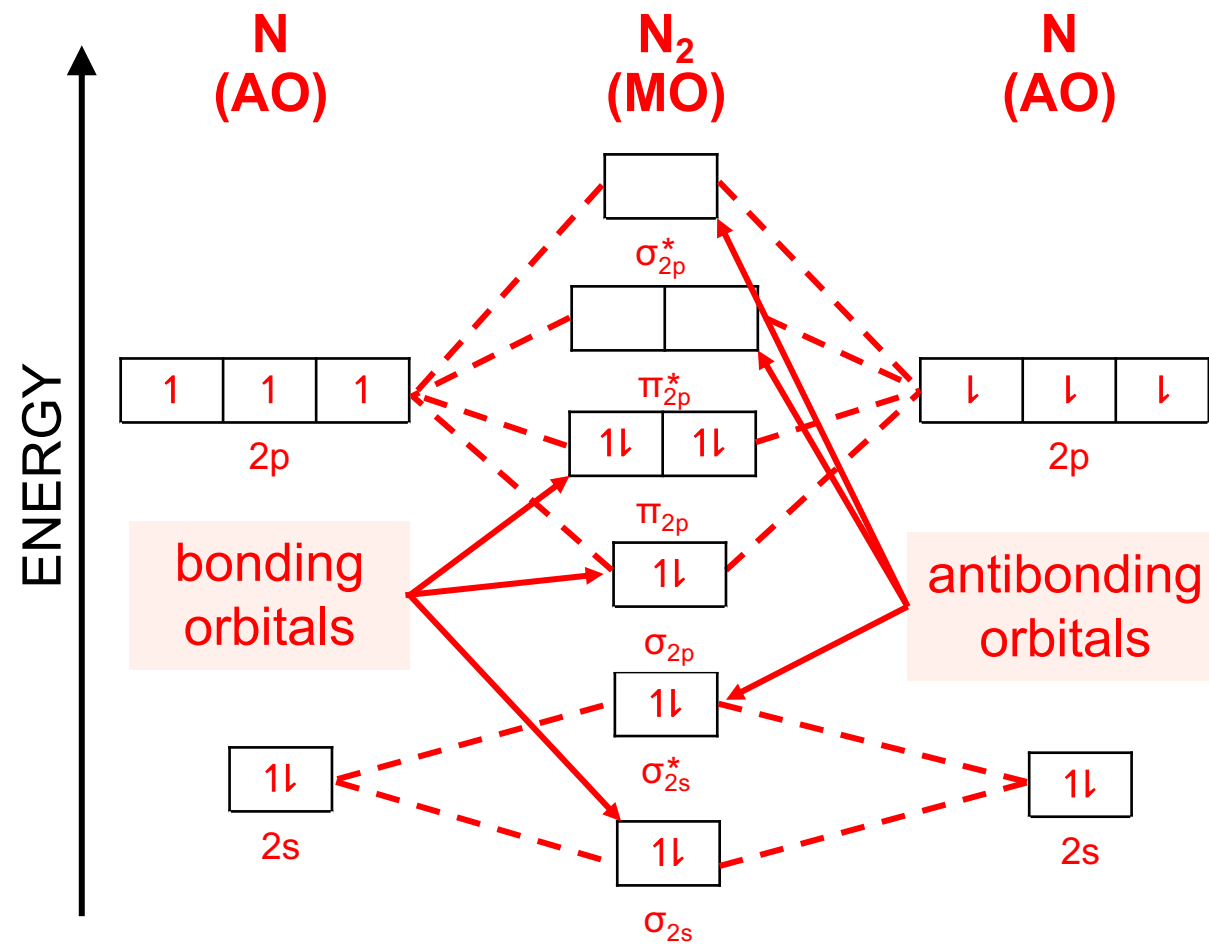
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BO = 1/2 [bonding e<sup>-</sup> – antibonding e<sup>-</sup>]

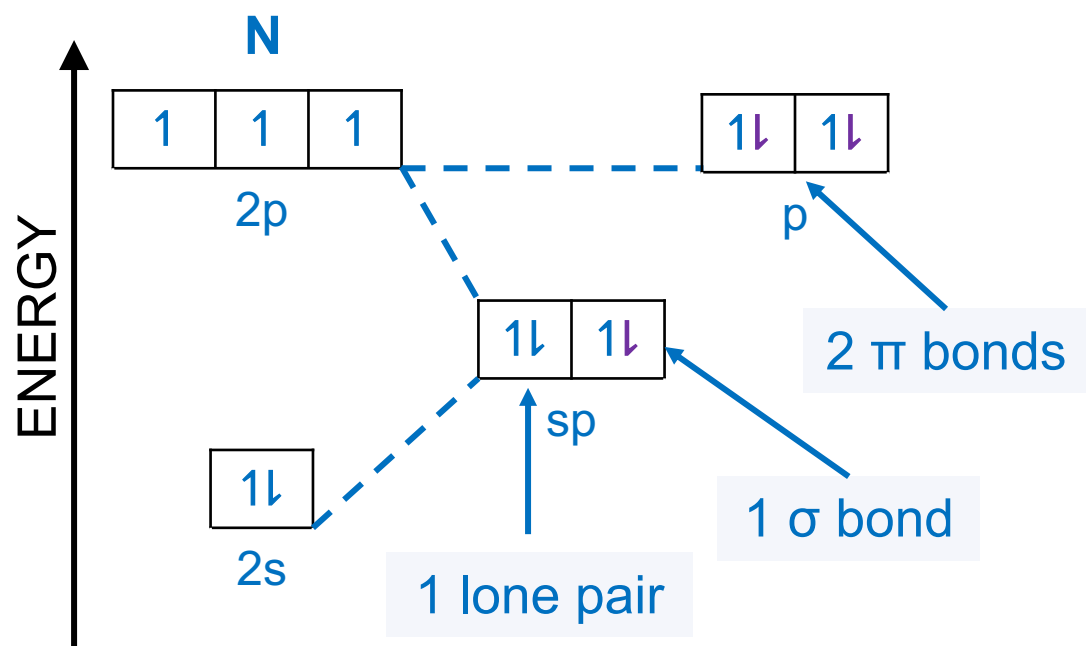




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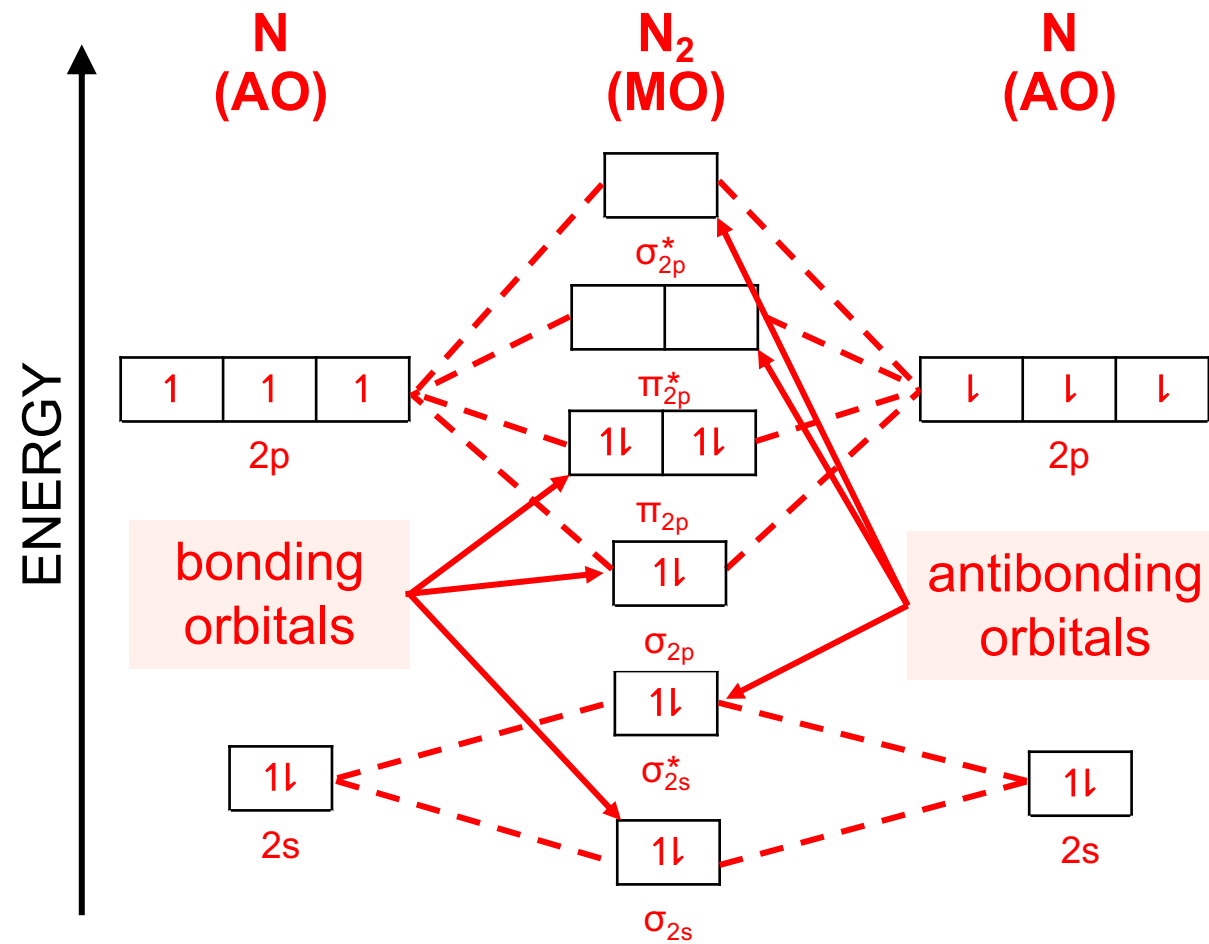
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BO =  $\frac{1}{2} [8 e^- - 2 e^-] = 3$  (triple bond)



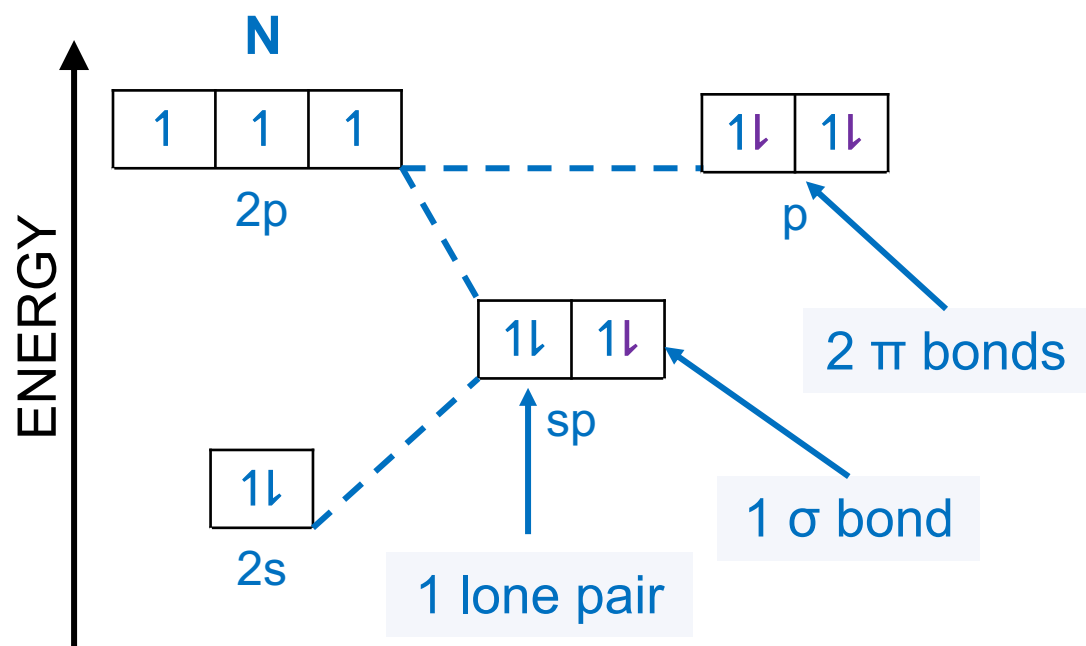
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**DIAMAGNETIC**

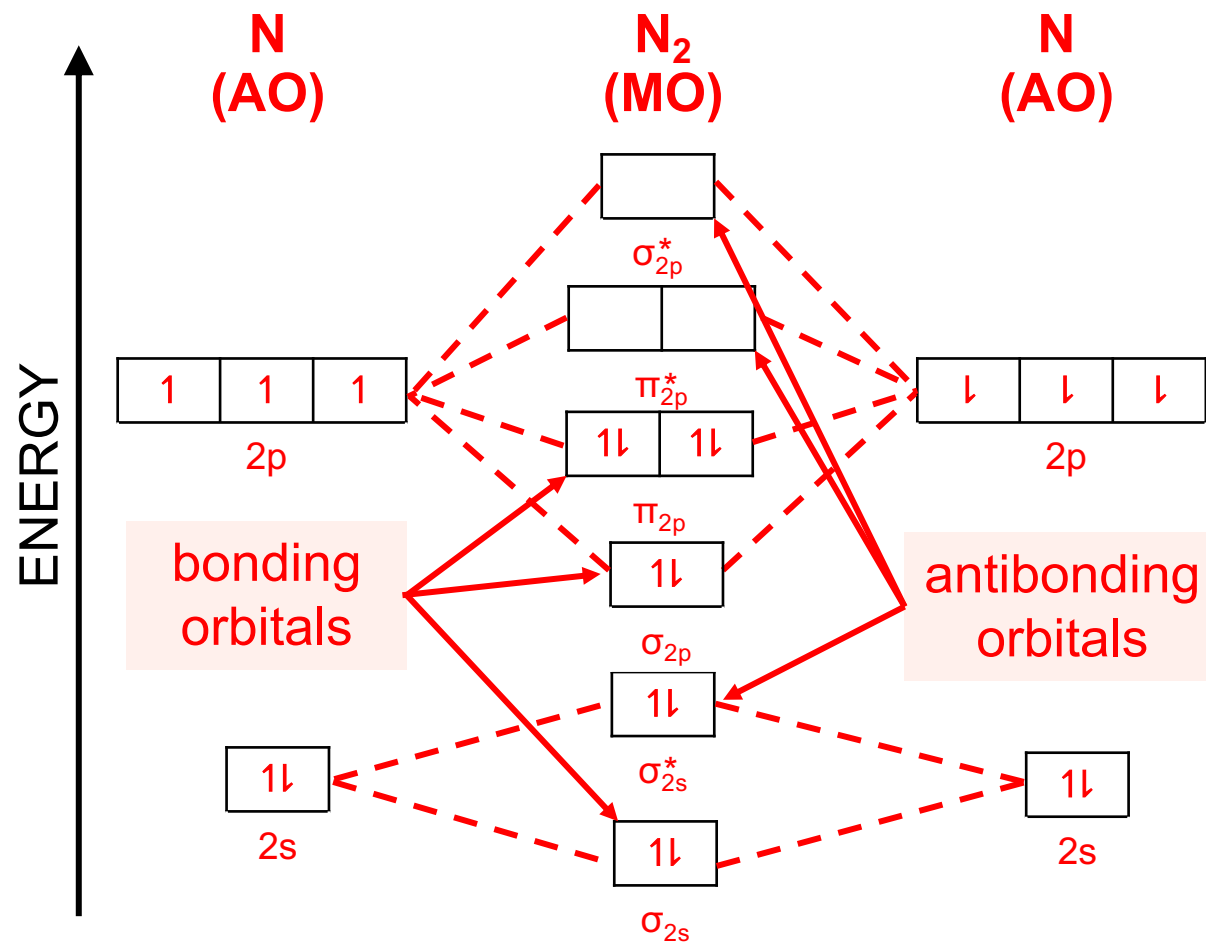
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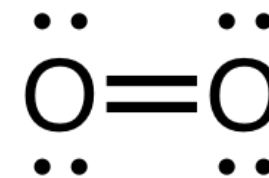
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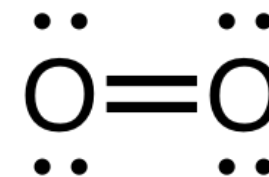
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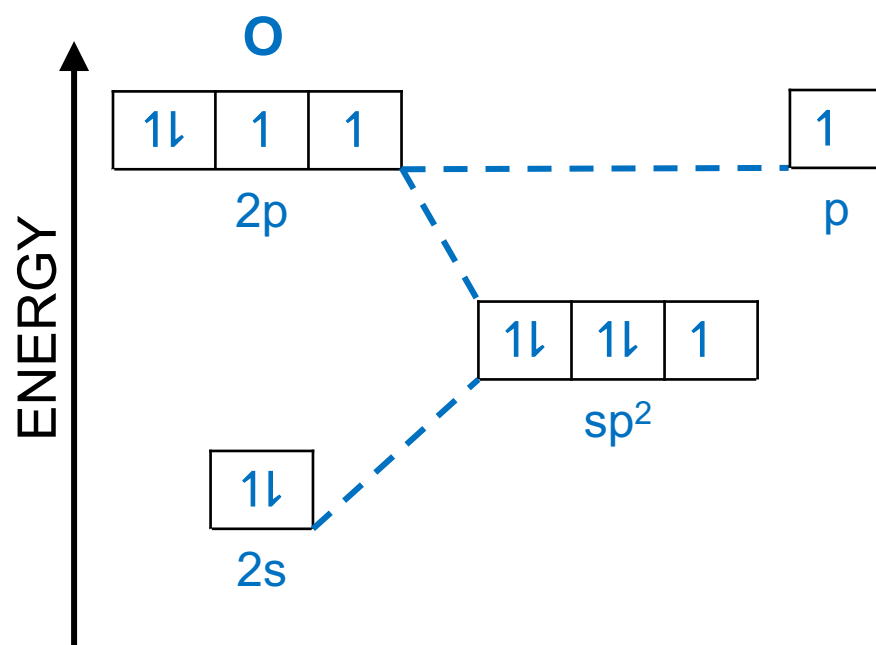
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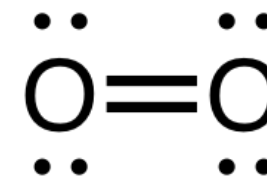
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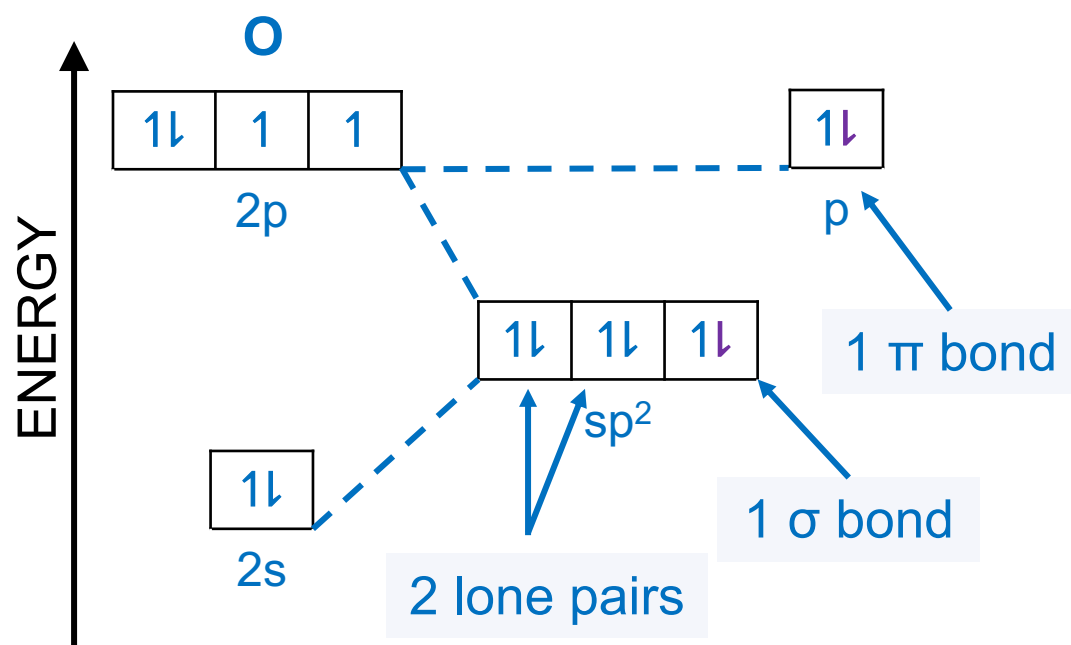
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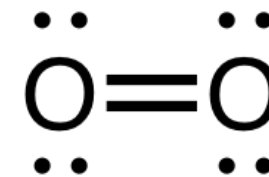
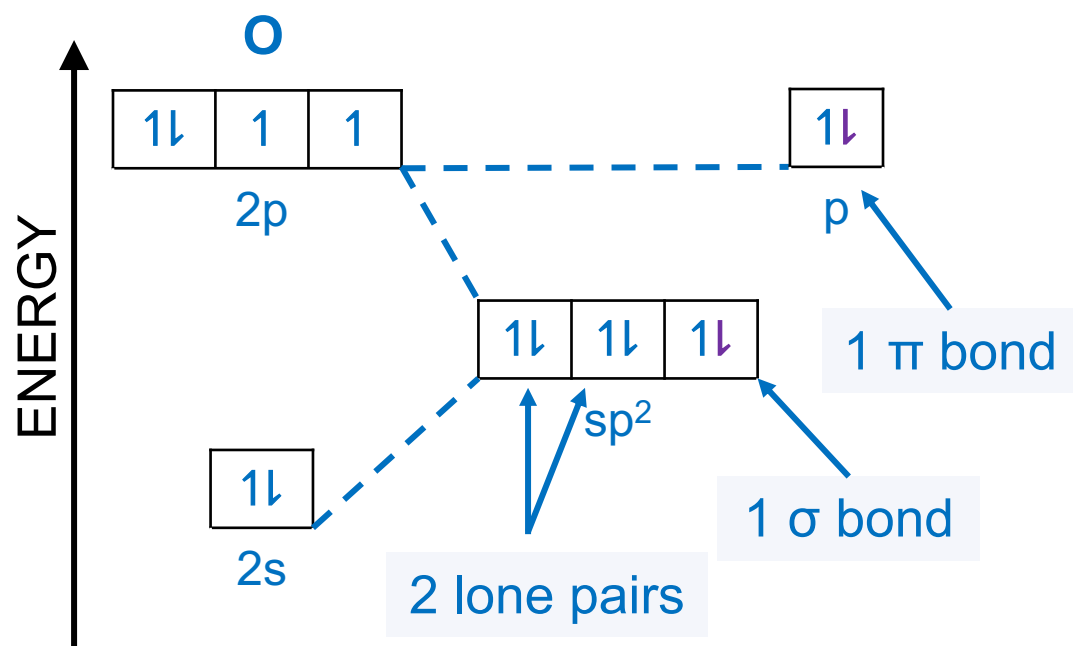
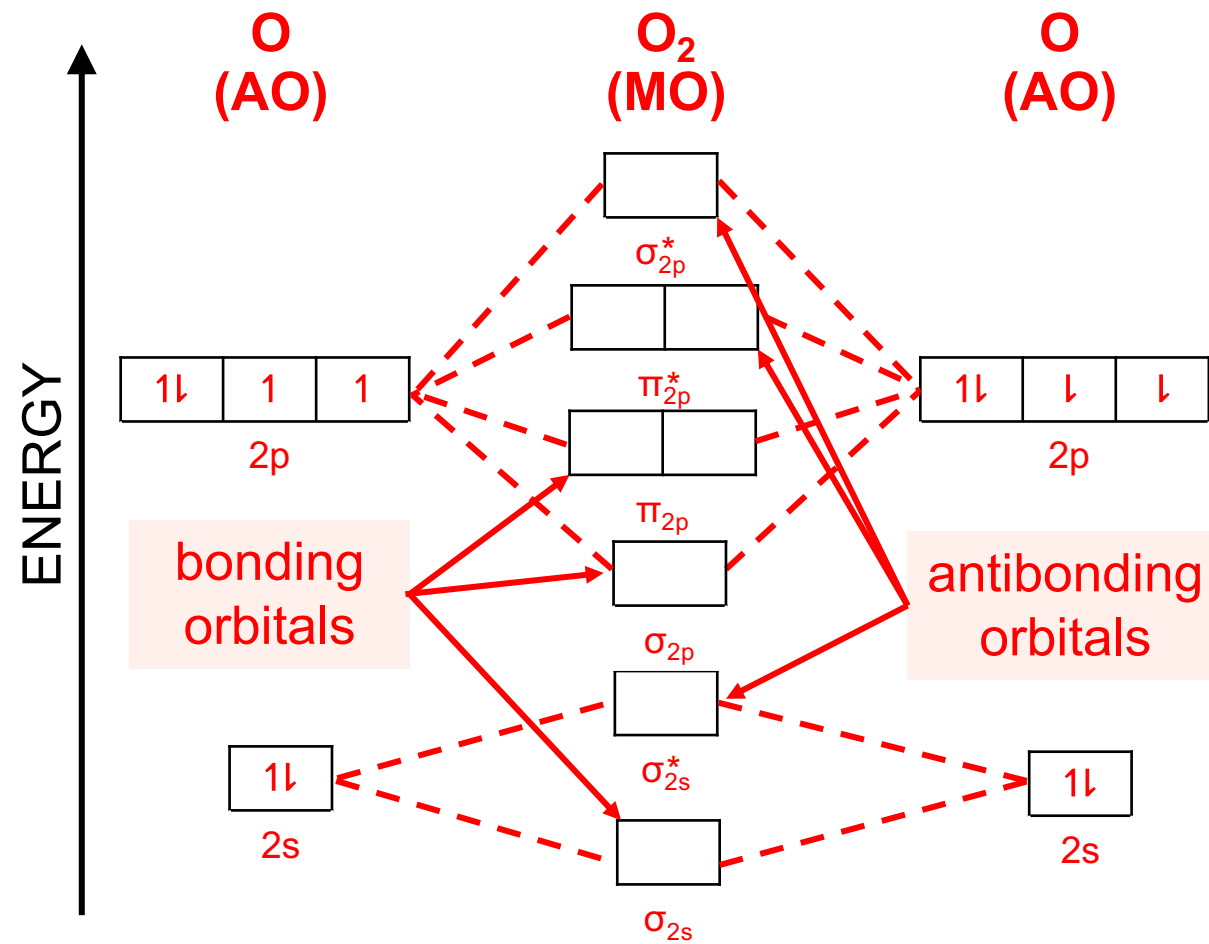
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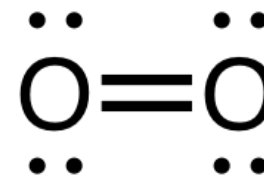
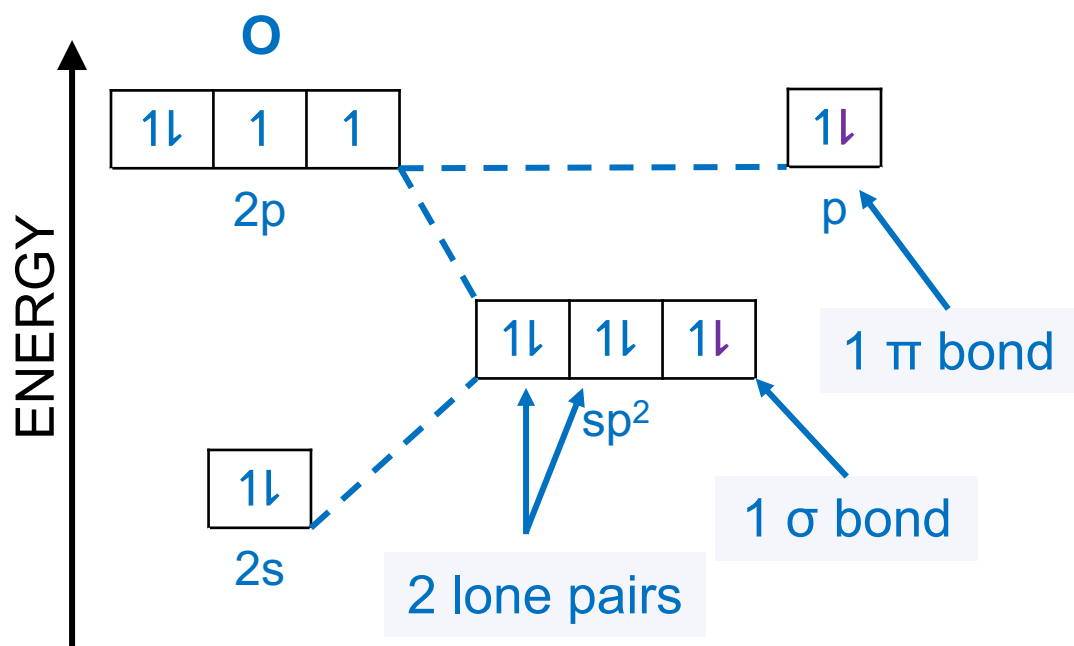
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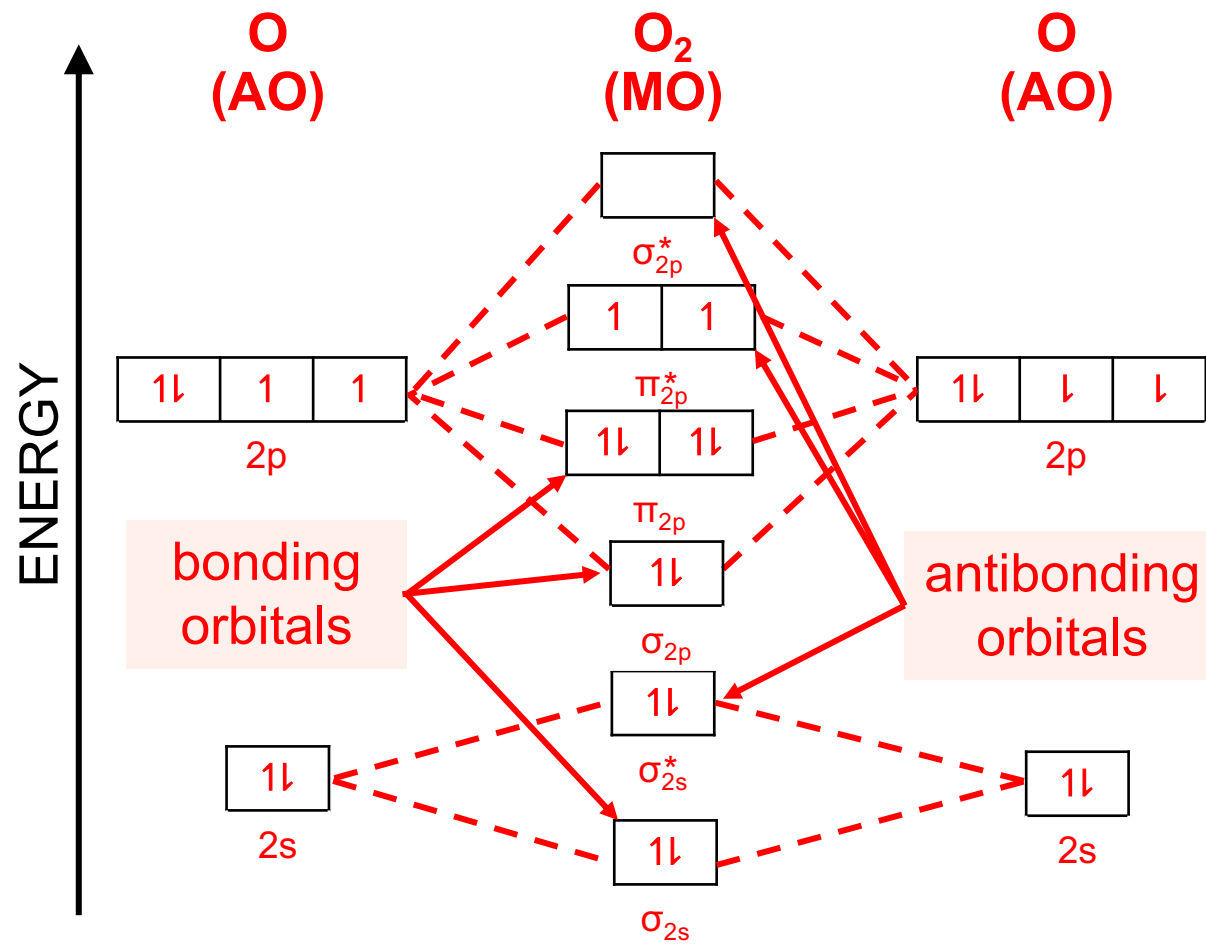
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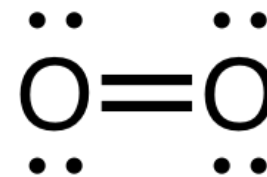
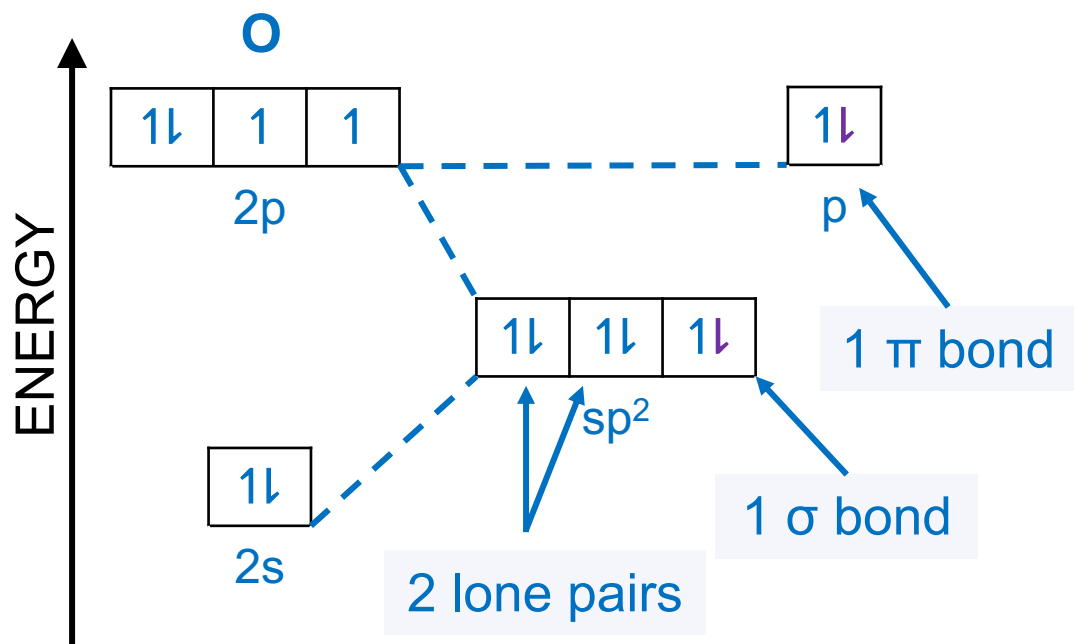
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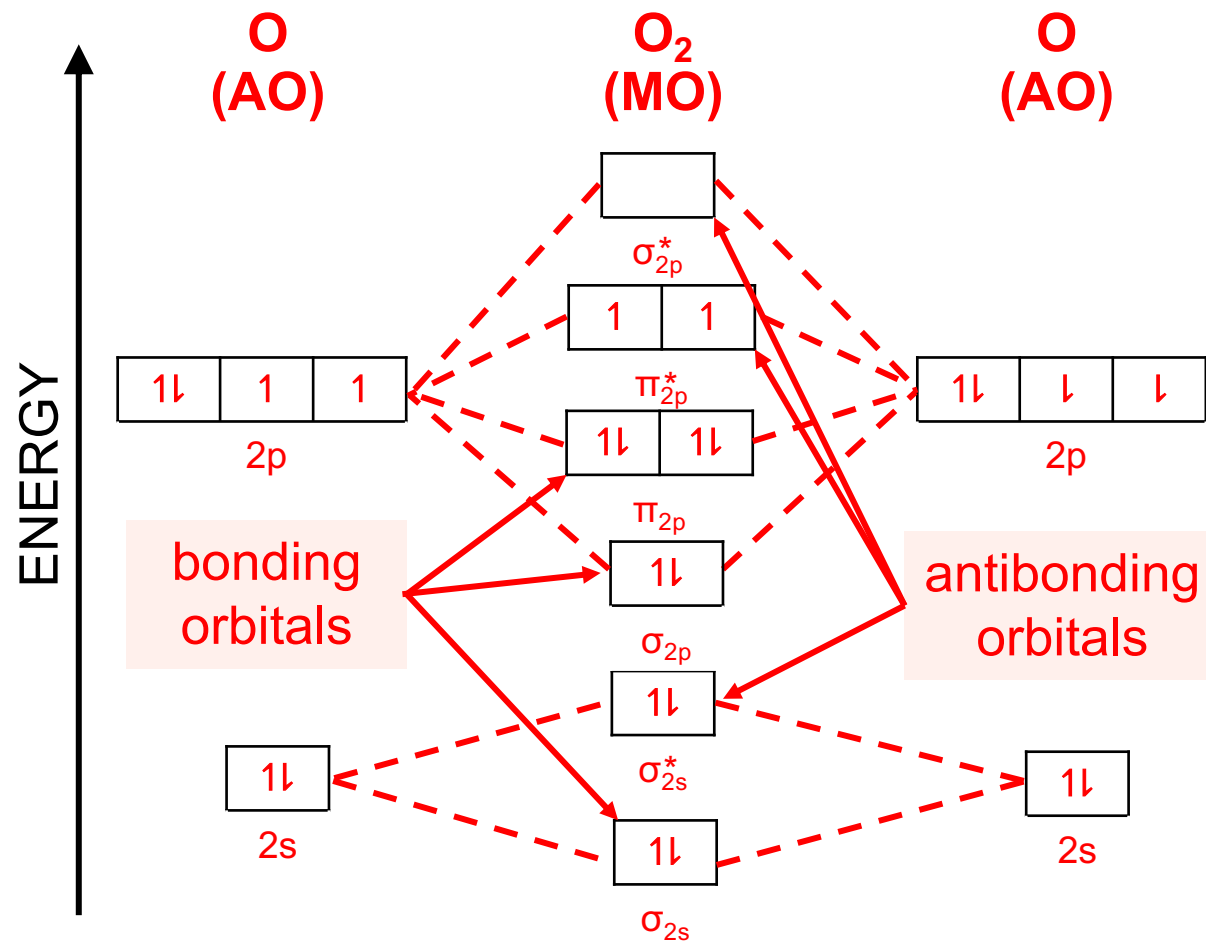
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*Molecular Orbital (MO) Theory*

$$BO = \frac{1}{2} [8 e^- - 4 e^-] = 3 \text{ (double bond)}$$

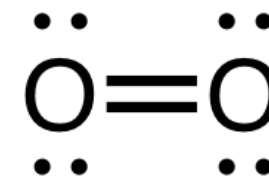
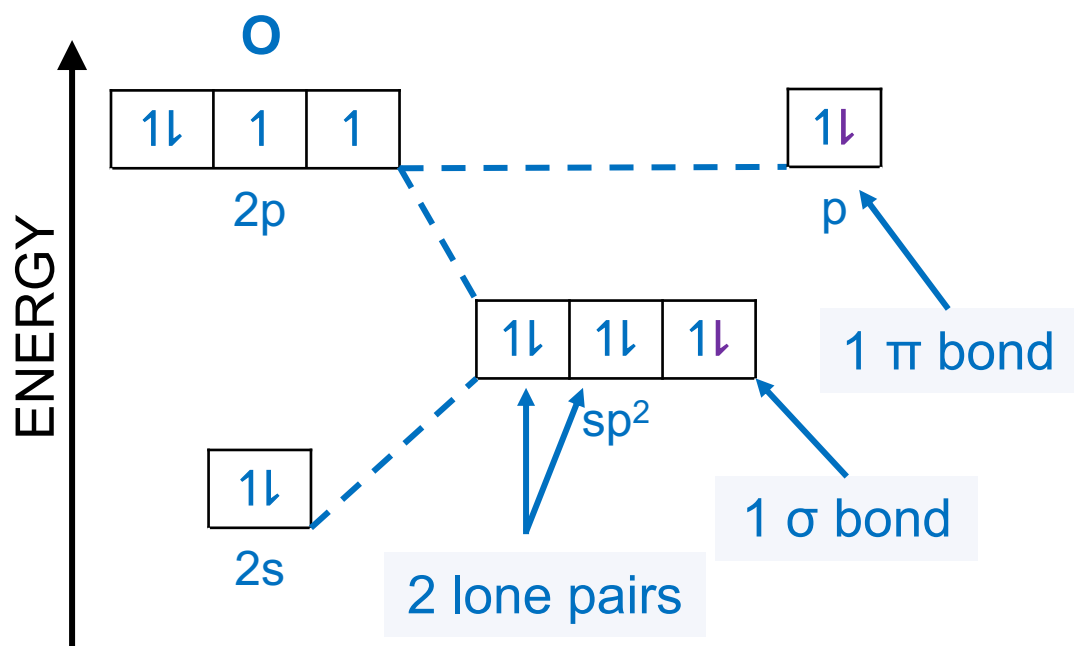




THE CASE OF O<sub>2</sub> (O = 1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup>)

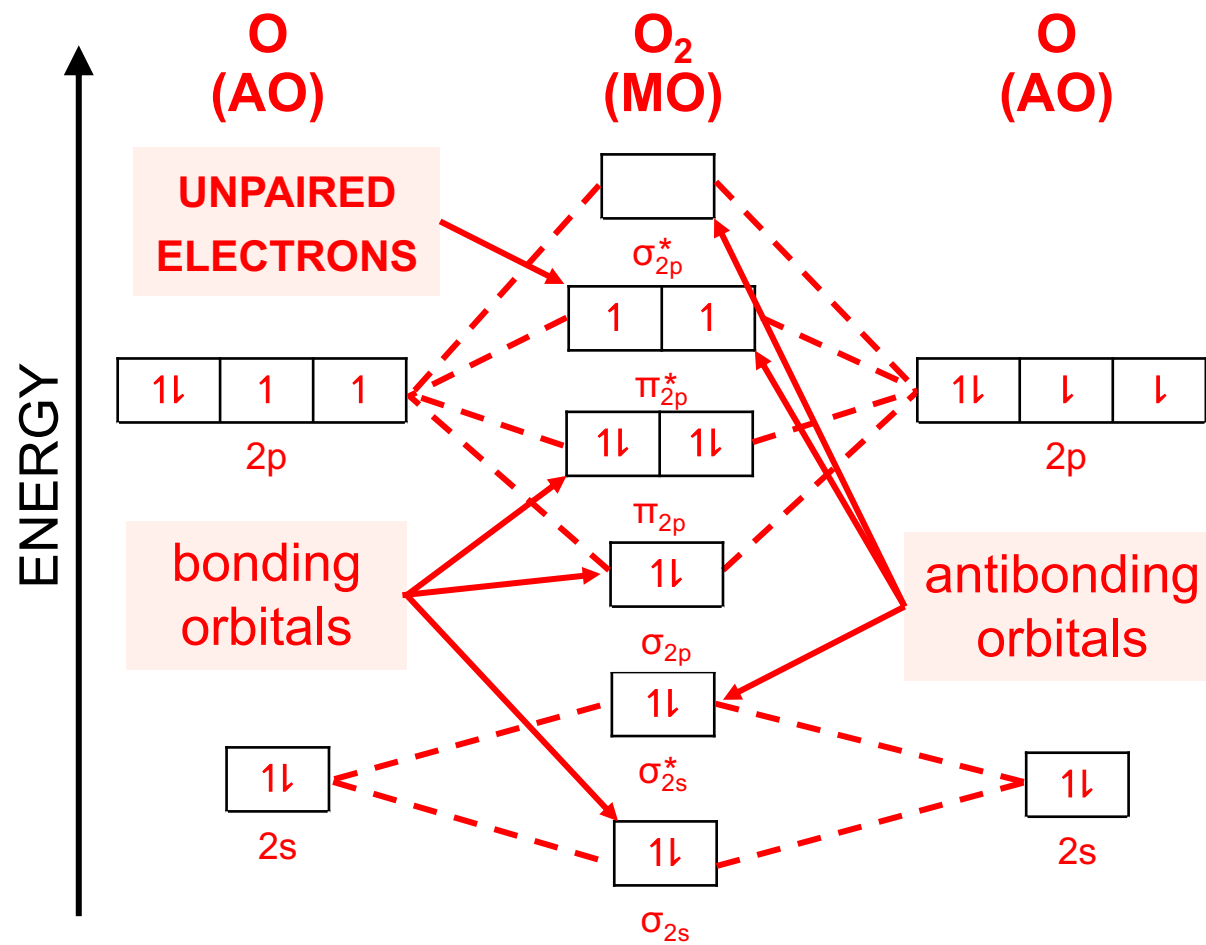
*Valence Bond (VB) Theory*

Each O atom is sp<sup>2</sup>-hybridized (SN = 3).  
The second O's electrons are in purple.



*Molecular Orbital (MO) Theory*

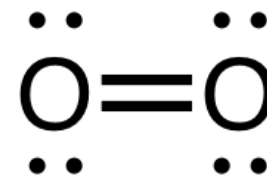
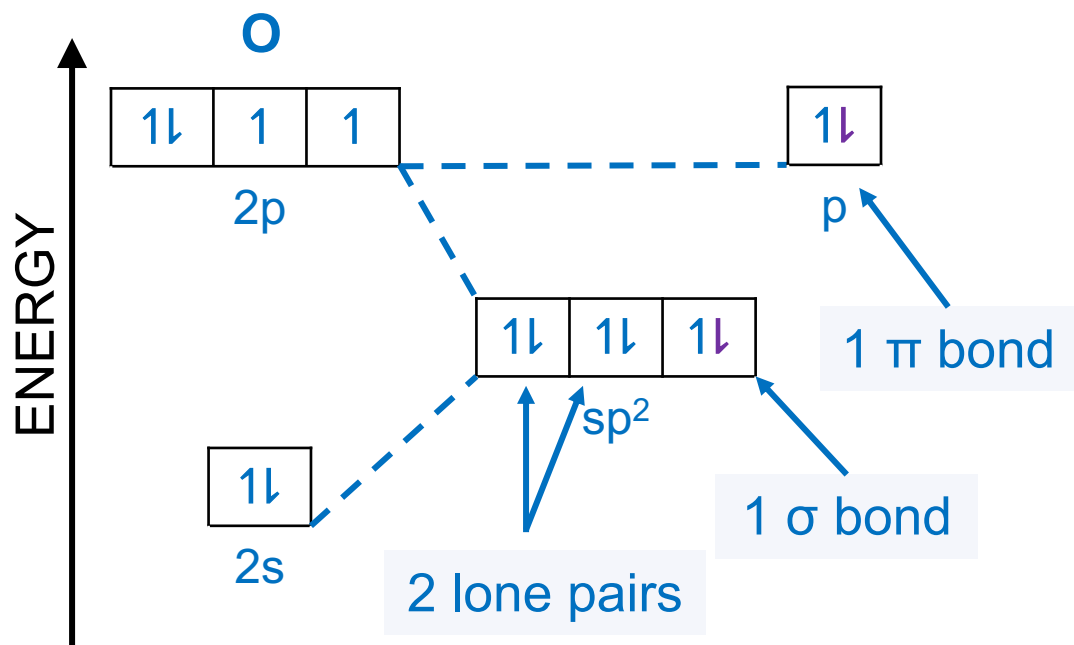
$$BO = \frac{1}{2} [8 e^- - 4 e^-] = 3 \text{ (double bond)}$$



THE CASE OF O<sub>2</sub> (O = 1s<sup>2</sup>2s<sup>2</sup>2p<sup>4</sup>)

*Valence Bond (VB) Theory*

Each O atom is sp<sup>2</sup>-hybridized (SN = 3).  
The second O's electrons are in purple.



PARAMAGNETIC

*Molecular Orbital (MO) Theory*

$$BO = \frac{1}{2} [8 e^- - 4 e^-] = 2 \text{ (double bond)}$$

