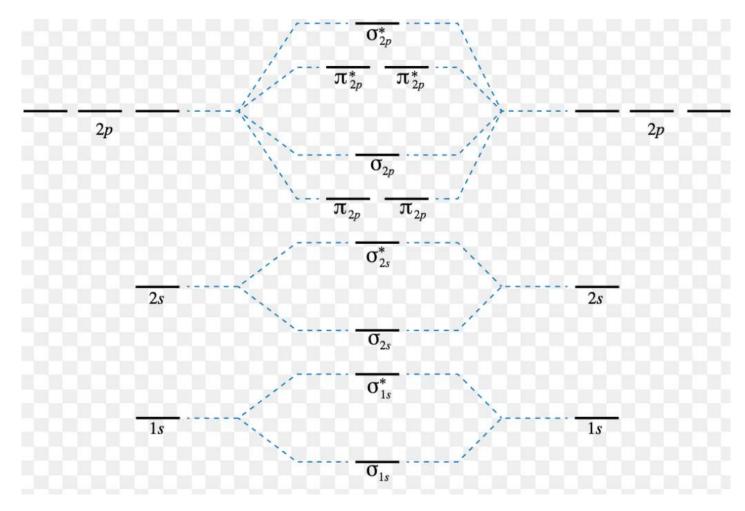
WELCOME

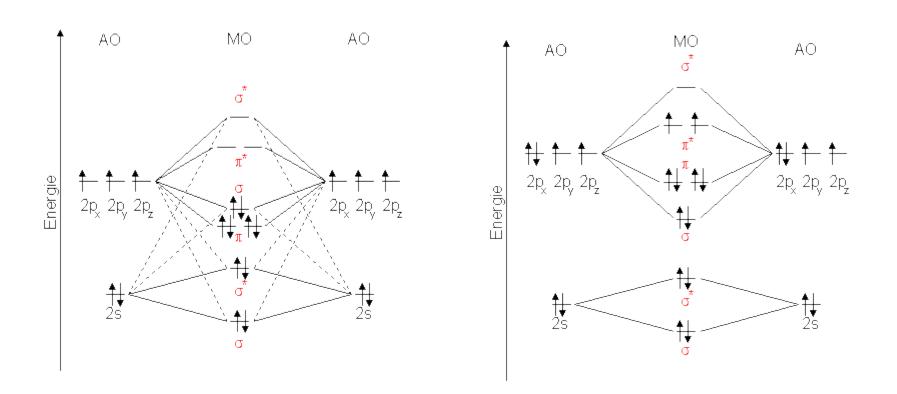
MOLECULAR ORBITAL THEORY

Moly PP Chemistry

ENERGY LEVEL DIAGRAMS FOR MOLECULAR ORBITALS

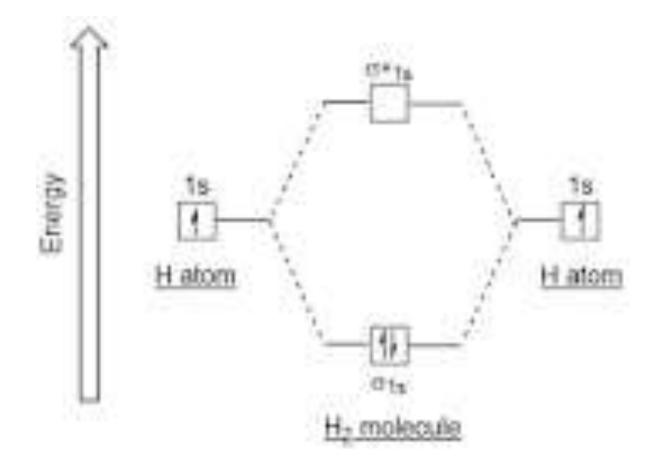


Why is the σ -MO formed by the 2p AOs energetically above the π -MO for N2 but not for O2



- All the elements in the second period before oxygen have the difference in energy between the 2s and 2p orbital small enough, so that s-p mixing (combination) can occur lowering the energy of the $\sigma(2s)$ and $\sigma^*(2s)$ and increasing the energy of the $\sigma(2p)$ and $\sigma^*(2p)$ molecular orbitals.
- By moving towards right in a period, the s orbital gets more stabilized than the p orbital and the difference in their energies increases, making the s-p mixing for oxygen much smaller.

MOLECULAR ORBITALELECTRONIC CONFIGURATIONS OF DIATOMIC MOLECULES



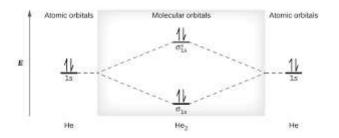
BOND ORDER CALCULATION & ITS SIGNIFICANCE

- Bond order = [(Number of electrons in bonding molecules) - (Number of electrons in antibonding molecules)]/2.
- Bond order and bond length indicate the type and strength of <u>covalent bonds</u> between atoms.
- Bond order and length are inversely proportional to each other: when bond order is increased, bond length is decreased.

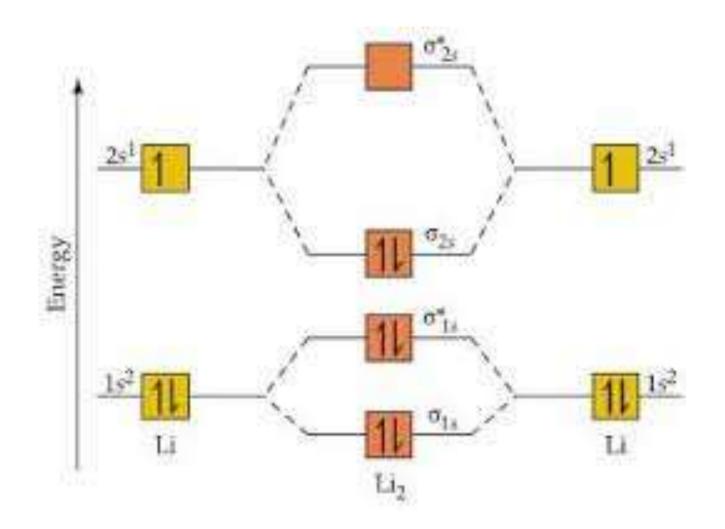
BOND ORDER VALUE

- 0: No bond
- 1: Single bond
- 2: double bond
- 3: triple bond

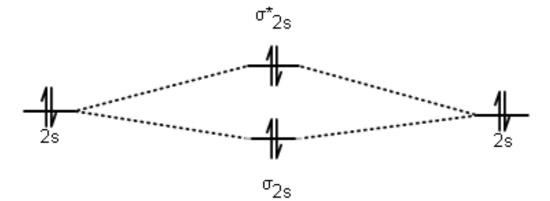
MO DIAGRAM OF HELIUM MOLECULE

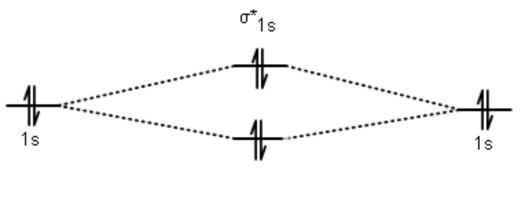


MO DIAGRAM OF LITHIUM MOLECULE



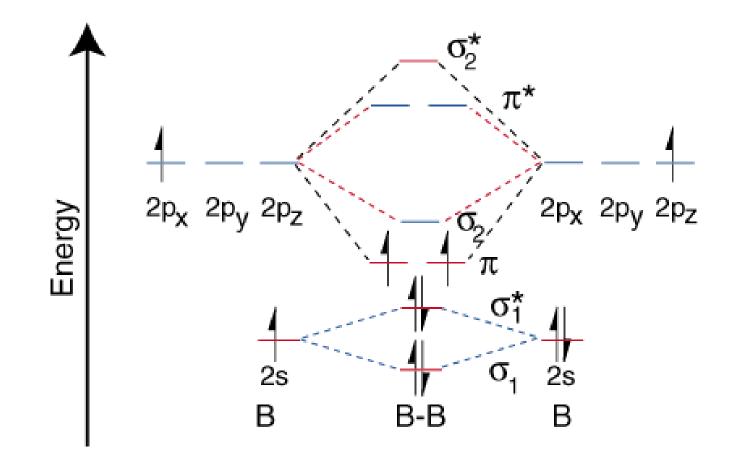
MO DIAGRAM OF BERILLIUM



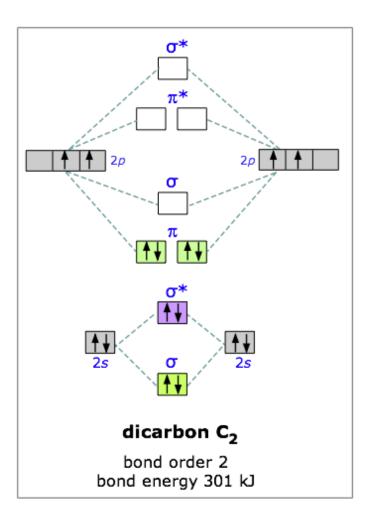


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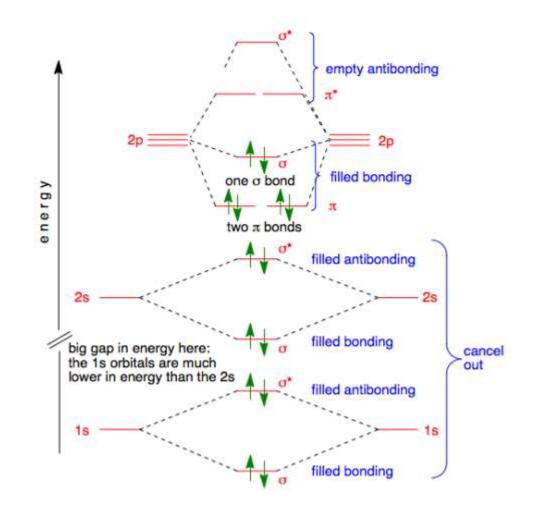
MO DIAGRAM OF BORON MOLECULE



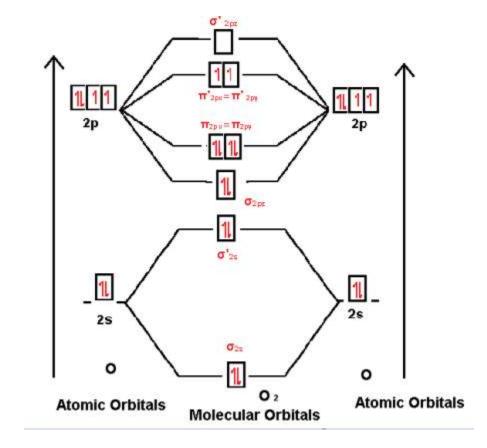
MO DIAGRAM OF CARBON MOLECULE



MO DIAGRAM OF NITROGEN MOLECULE



MO DIAGRAM OF OXYGEN MOLECULE



MO DIAGRAM OF FLUORINE MOLECULE

