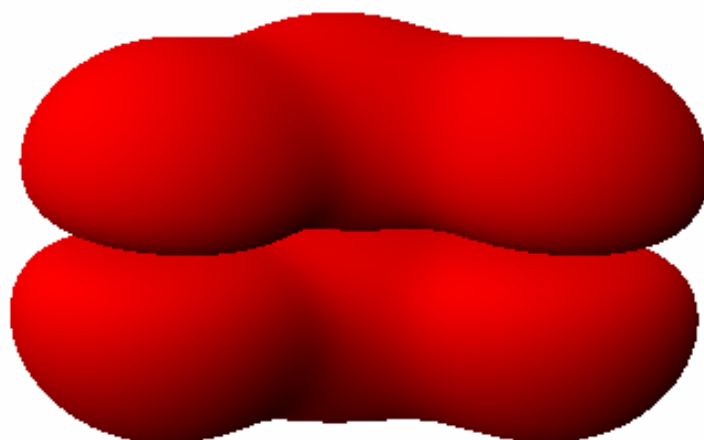


MO Description of Pi-Delocalized Systems

- L MO theory has no difficulty explaining the π -delocalized electron density implied by resonance forms, which VB theory cannot easily represent.



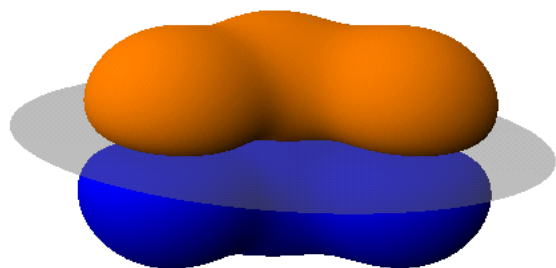
π electron density of O₃

Pi MOs of Ozone, O₃

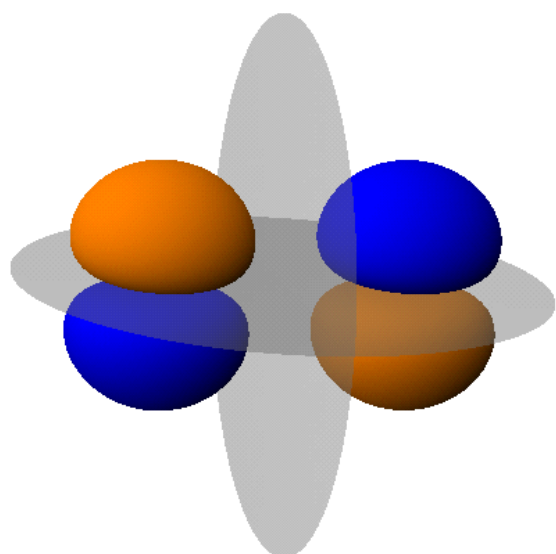
- U The three $2p$ orbitals perpendicular to the molecular plane combine to form three π MOs:
 1. π – bonding MO
 2. π^n – nonbonding MO
 3. π^* – antibonding MO

- U A non-bonding MO neither builds nor destroys bonding between the oxygen atoms.

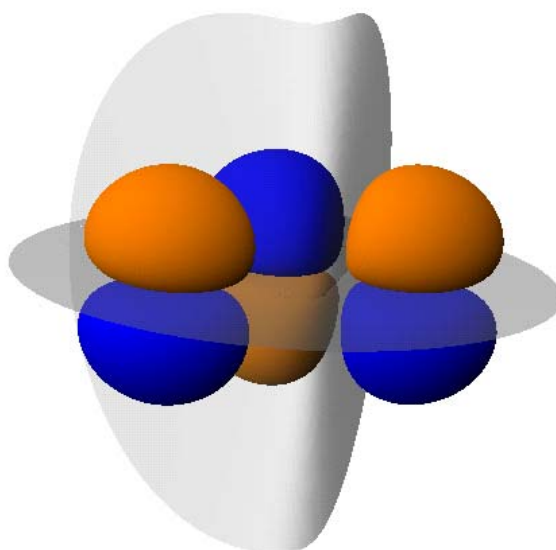
Pi MOs of Ozone, O₃



π (bonding)



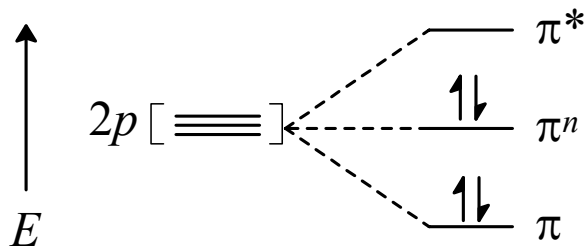
π^n (nonbonding)



π^* (antibonding)

Pi MO Energy Level Scheme for O₃

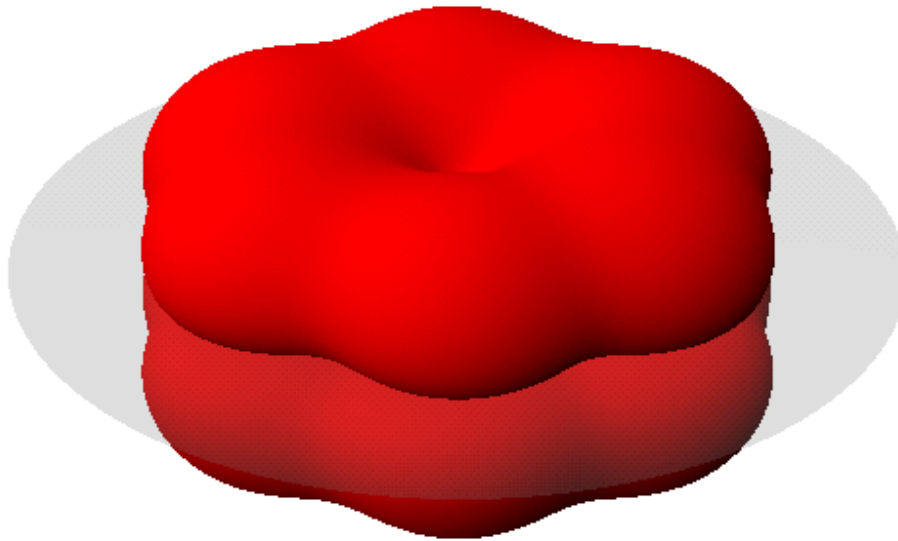
- U The π system has two pairs of electrons, one pair in the π MO, and the other in the π^n non-bonding MO.



- U The configuration $(\pi)^2$ adds a bond order of 1 across the two O–O bonds (i.e., 0.5 to each bond).
- U When this is added to the sigma bond between each oxygen pair, the O–O bond order becomes 1.5.
- U The configuration $(\pi^n)^2$ neither adds nor subtracts from the overall strength of the bonds.

Pi MOs of Benzene, C₆H₆

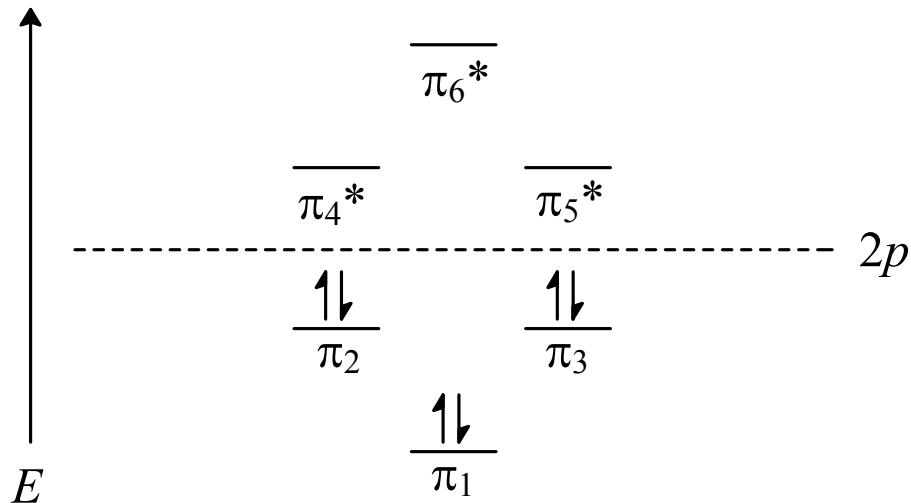
- U C₆H₆, has three pairs of electrons delocalized in a π system extending around the hexagonal ring.



π electron density of benzene

- U The six $2p$ orbitals perpendicular to the ring on the six carbon atoms combine to form three bonding (π_1 , π_2 , π_3) and three antibonding (π_4^* , π_5^* , π_6^*) MOs.

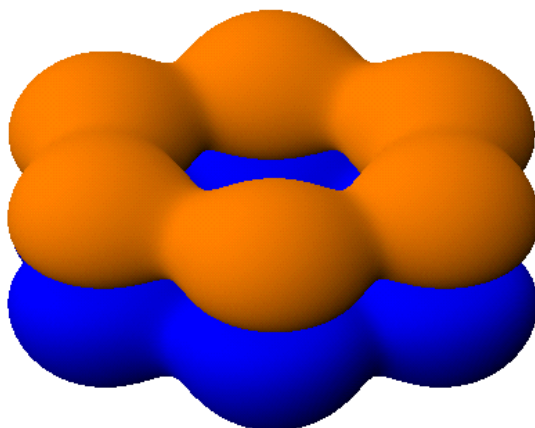
Pi MO Energy Level Scheme for Benzene, C₆H₆



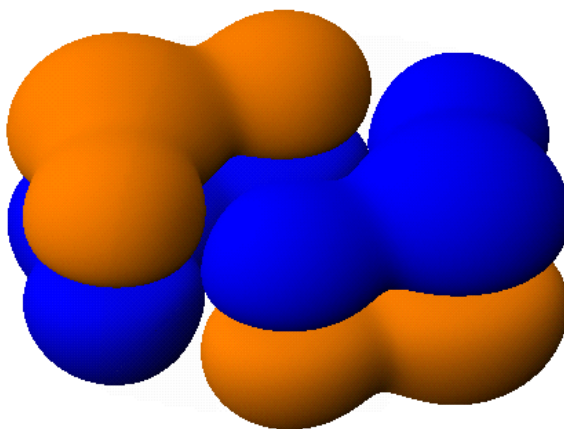
- U Three pairs in bonding MOs add a total of three bond orders over six C–C linkages, or 0.5 for each.
- U When this is added to the sigma bond between each carbon pair, the C–C bond order becomes 1.5.

Occupied Bonding π MOs of Benzene, C_6H_6

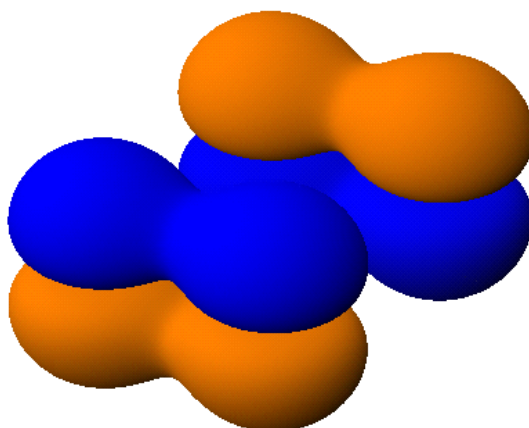
π_1



π_2

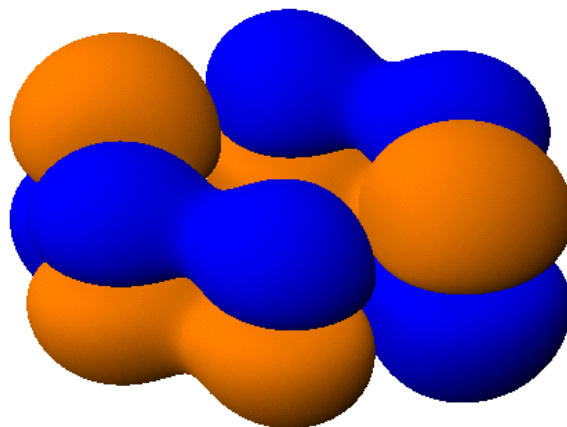


π_3

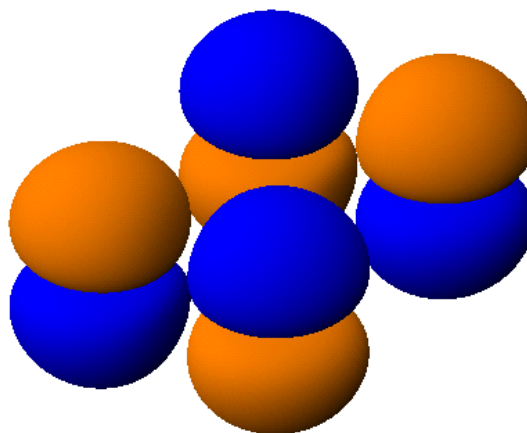


Unoccupied Antibonding π^* MOs of Benzene, C_6H_6

π_4^*



π_5^*



π_6^*

