

Pi-Type Pairwise Orbital Combinations

- ✓ Continue to follow the convention for combining orbital pairs
 - Bring orbitals together along their positive x-axes
 - Rotate atom 2 by 180° about its z or y axis
 - Orbitals of the same sign become bonding
 - Orbitals of opposite sign become antibonding
- ✓ Identify all the pi-type combinations
 - Side-by-side
 - Parallel (or nearly so)
 - Pairs of 2p atomic orbitals



Identify All of the pi-type Combinations

atom 2 \ atom 1	2s	-2s	2p _x	-2p _x	2p _y	-2p _y	2p _z	-2p _z
2s								
-2s								
2p _x								
-2p _x								
2p _y								
-2p _y								
2p _z								
-2p _z								

SHEET #1

Instructions: (Part 1) For each symmetry allowed combination, draw the orbital that results when the two atoms are brought together along the the x-axis (calling the internuclear axis the x-axis). See the example below:

atom 1 atom 2

atom 1 atom 2

Instructions: (Part 2) Draw an outline around the group of orbital combinations that are not allowed to interact because of symmetry reasons. Write the label "symmetry forbidden" in large letters inside this zone.

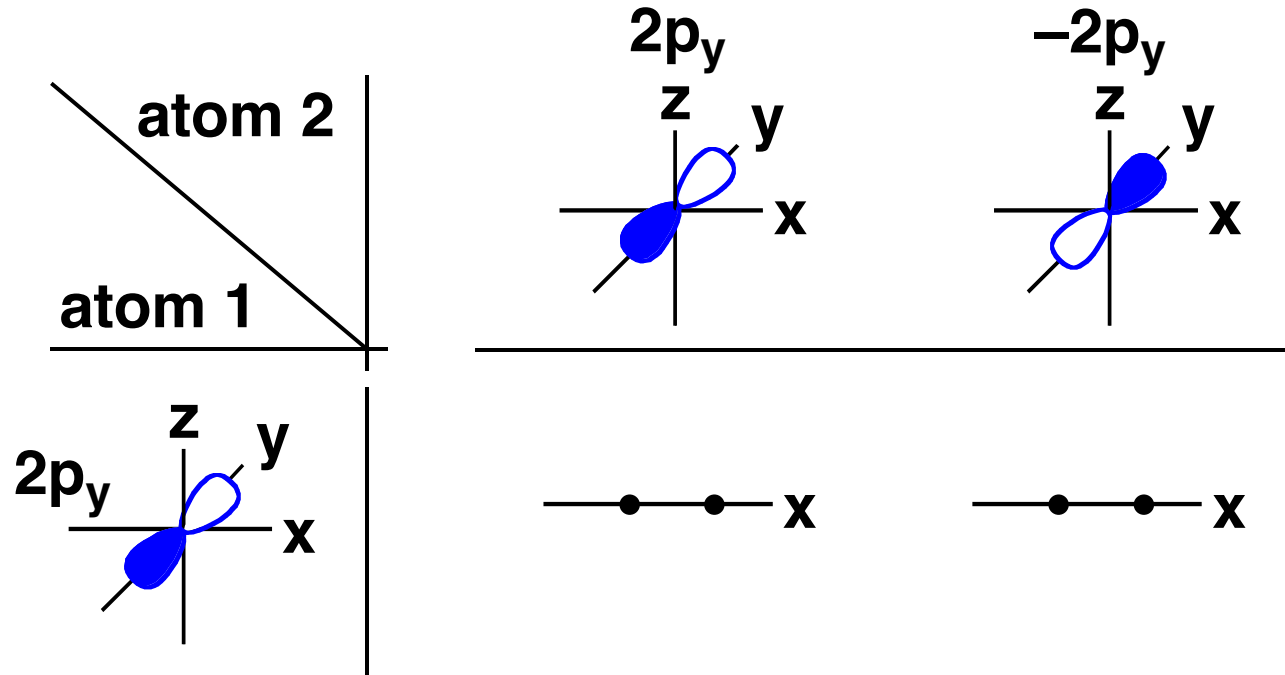
Bringing orbitals together from two different atoms → making MOs

- some orbital combinations interact in such a way as to concentrate the electron density between the nuclei (**bonding interactions**)
- some orbital combinations interact in such a way as to deplete the electron density between the nuclei (**antibonding interactions**)
- some orbital combinations interact in such a way as to neither concentrate nor deplete the electron density between the nuclei (**nonbonding interactions**)

See: Molecular Orbitals (N₂) at <http://www.shef.ac.uk/chemistry/orbitron/>

Instructions: (Part 3) For each allowed combination, add one of the following labels ($\sigma_s, \sigma_s^*, \sigma_p, \sigma_p^*, \sigma_{s/p}, \sigma_{s/p}^*, \pi_y, \pi_y^*, \pi_z, \pi_z^*$) where * denotes an antibonding interaction.

Side-by-Side Pairwise Combinations



$$2p_y + 2p_y = \pi_y$$

$$2p_y - 2p_y = \pi_y^*$$