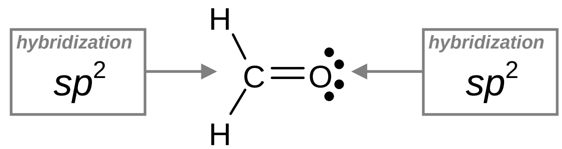
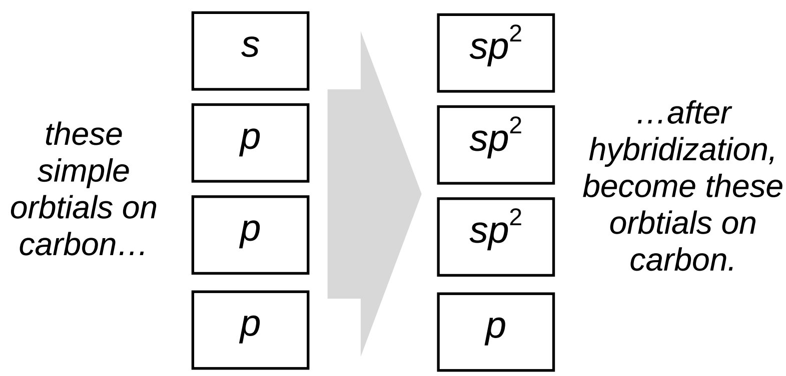
Chemistry 2331H Tuesday, September 24

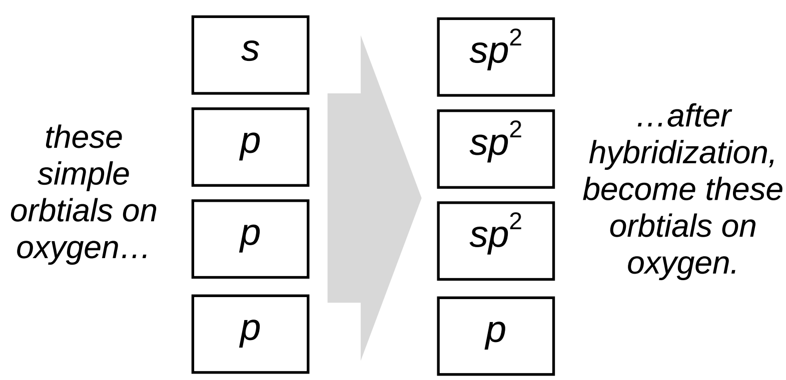
Workshop 7 Solutions
Molecular Orbitals

a) At each atom, hybridization is determined by (number of σ bonds) + (number of lone pairs). Carbon has three σ bonds and no lone pairs, so three atomic orbitals—an *s* and two *p*'s—contribute to three sp^2 hybrid orbitals. Oxygen has one σ bond and two lone pairs, so it also has three sp^2 hybrid orbitals.

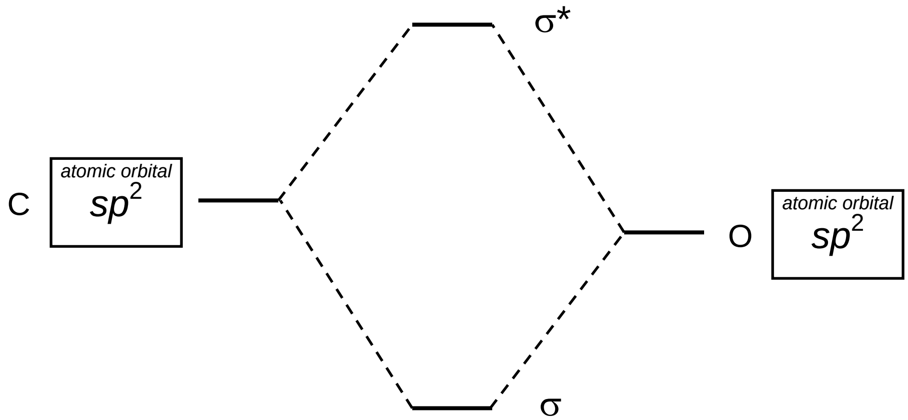


b) If carbon and oxygen are each sp^2-hybridized, then they each also have one *p* orbital left over, that remains a simple (unhybridized) orbital.



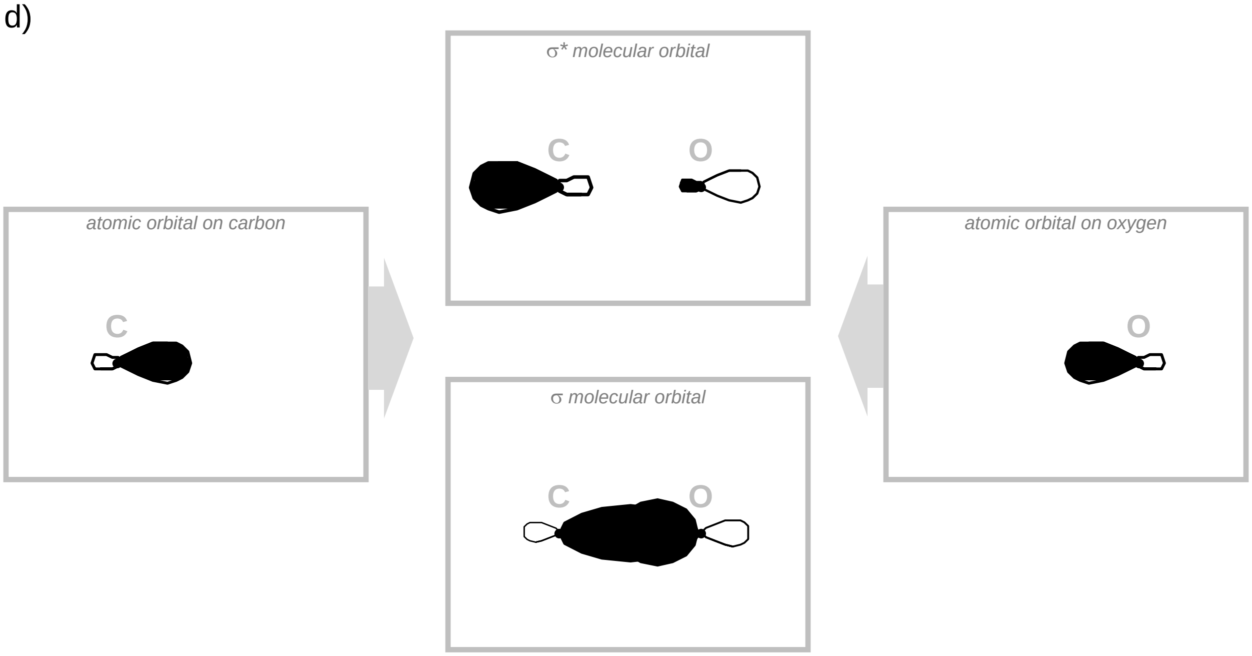


c)



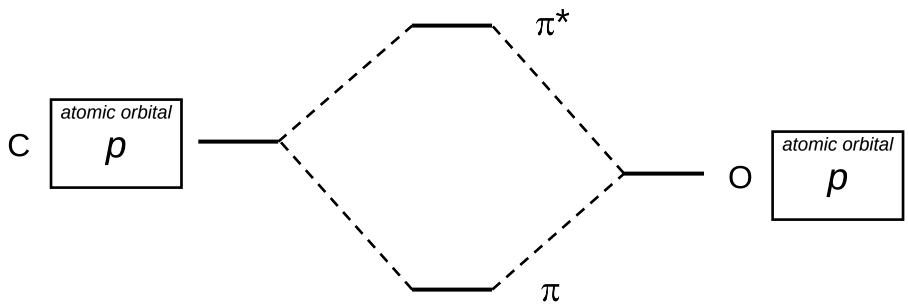
Why did I draw the starting oxygen orbital lower in energy than the starting carbon orbital? Oxygen is more electronegative, meaning electron density (a filled orbital) is more stable on oxygen than on carbon.

d)



The two molecular orbitals represent constructive and destructive combinations of the starting atomic orbitals. The σ molecular orbital is closer in energy to the O(sp^2) orbital than the C(sp^2) orbital, so it has more O(sp^2) character; the σ^* orbital is closer to C(sp^2), so it has more C(sp^2) character.

e)



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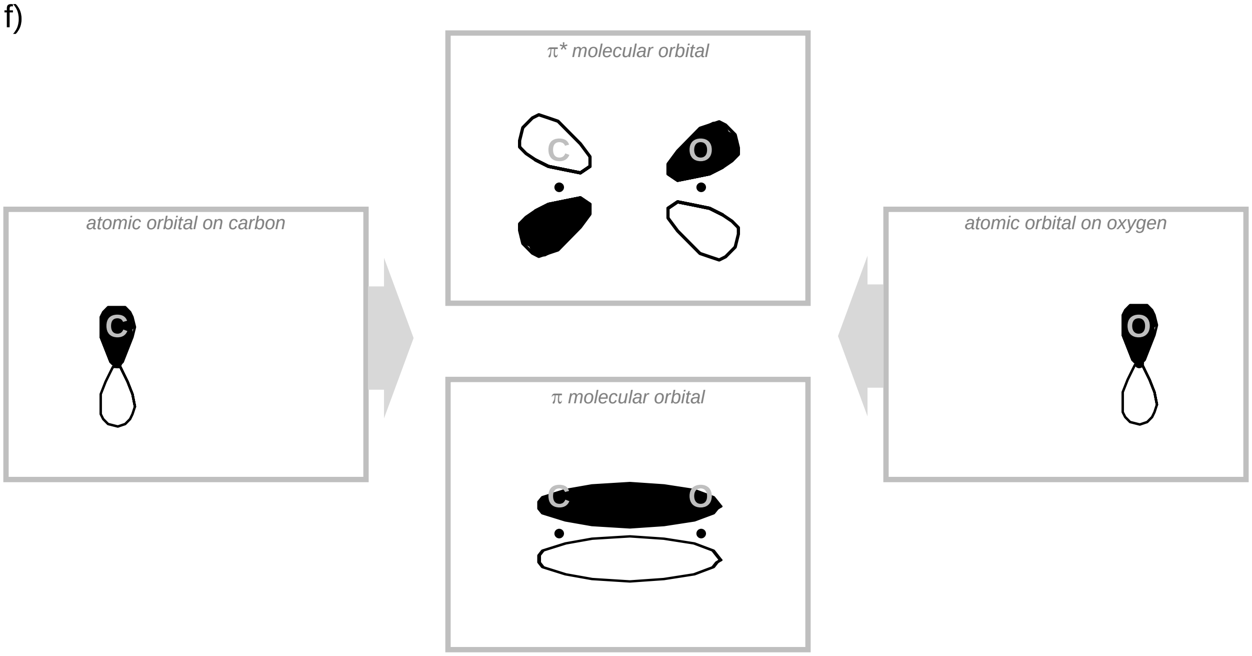
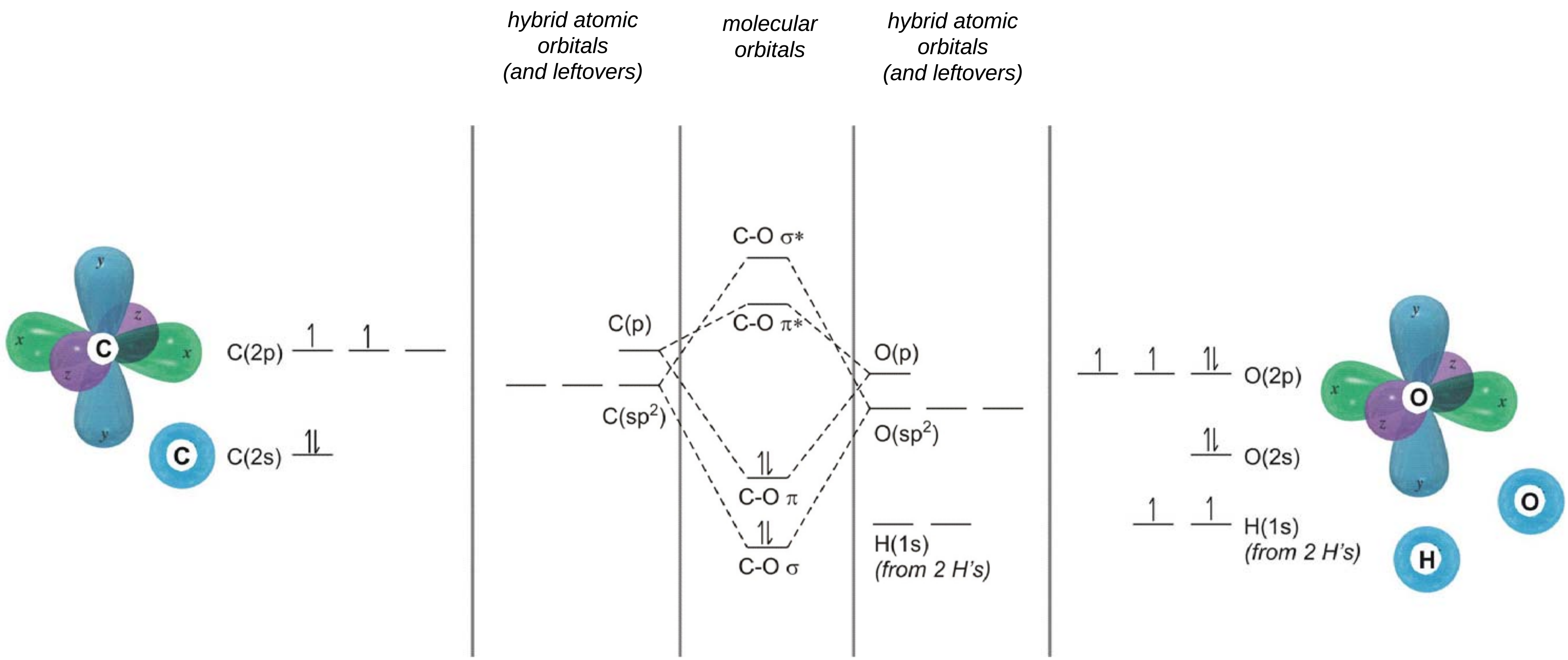
f)

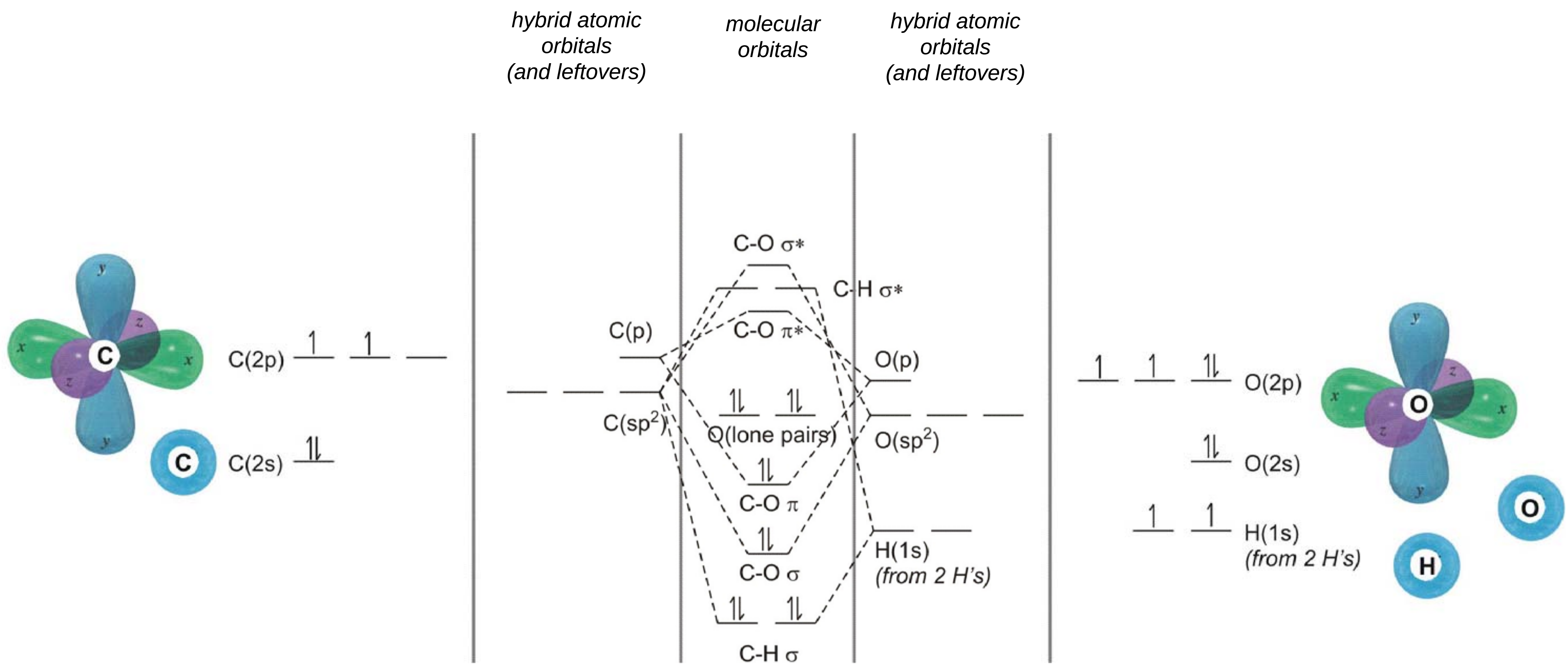


g) We still need to explain what happens to two sp^2 orbitals on carbon and two sp^2 orbitals on oxygen that we haven't used yet. Carbon makes two more σ bonds with two hydrogen atoms, so that's where each of the C(sp^2) orbitals goes. Oxygen doesn't have any bonds other than the C=O bond; its remaining electrons are lone pairs, and each lone pair will occupy one of the sp^2 atomic orbitals.

h and i) Next two pages.



hybrid atomic orbitals (and leftovers)
molecular orbitals
hybrid atomic orbitals (and leftovers)
C
C(2p)
C(2s)
C(p)
C(sp^2)
C-O σ*
C-O π*
C-O π
C-O σ
O(p)
O(sp^2)
H(1s) (from 2 H's)
O(2p)
O(2s)
H(1s) (from 2 H's)
O
H


hybrid atomic orbitals (and leftovers)
molecular orbitals
hybrid atomic orbitals (and leftovers)
C-O σ*
C-H σ*
C-O π*
C(p)
C(2p)
O(p)
O(2p)
C(sp²)
O(lone pairs)
O(sp²)
C(2s)
O(2s)
C-O π
C-O σ
H(1s)
(from 2 H's)
H(1s)
(from 2 H's)
C-H σ
C
C
O
O
H