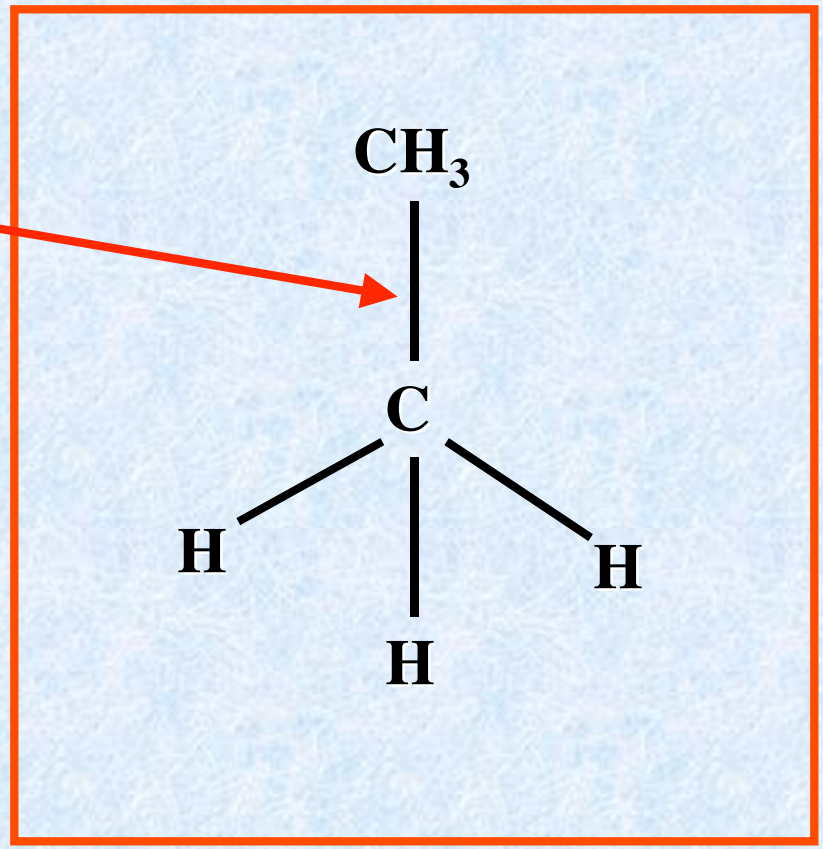
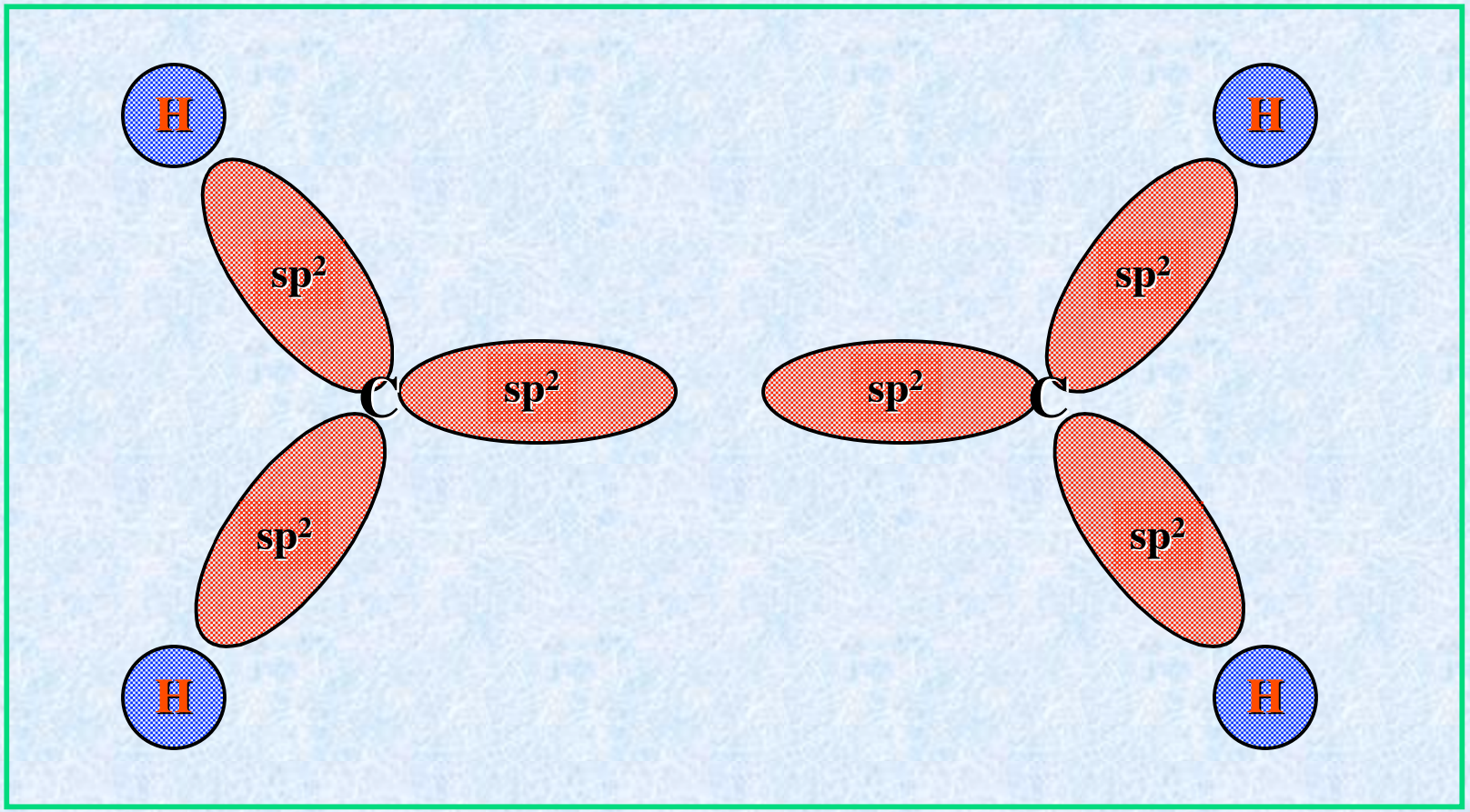
Single and Multiple Bonds in Carbon Compounds

sp^3 hybridization on C leads to 4 bonds. CH_4 is a good example. $CH_3(CH_3)$ is another example:

1 C-C sp^3/sp^3 bond



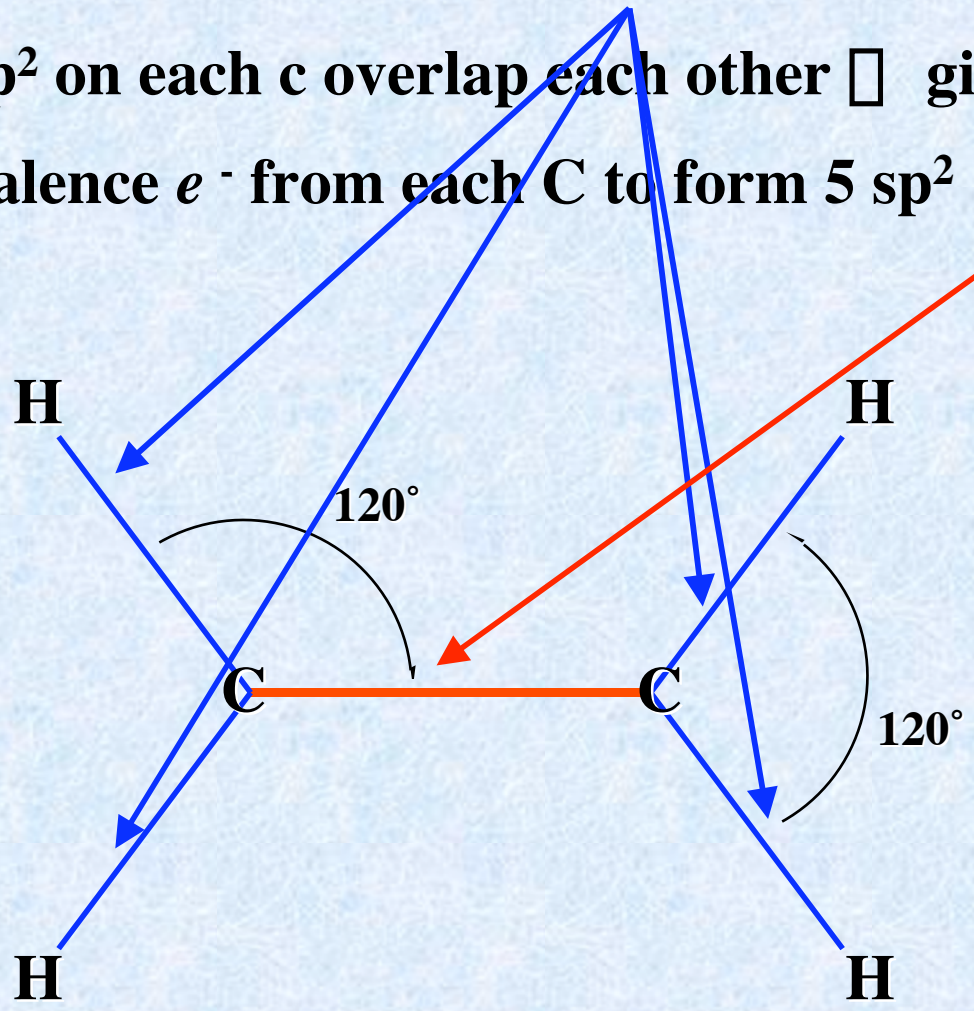
Carbon can also exhibit sp^2 hybridization: C_2H_4 (ethylene)



2 of sp^2 orbitals on each C form C-H bonds (total of 4)

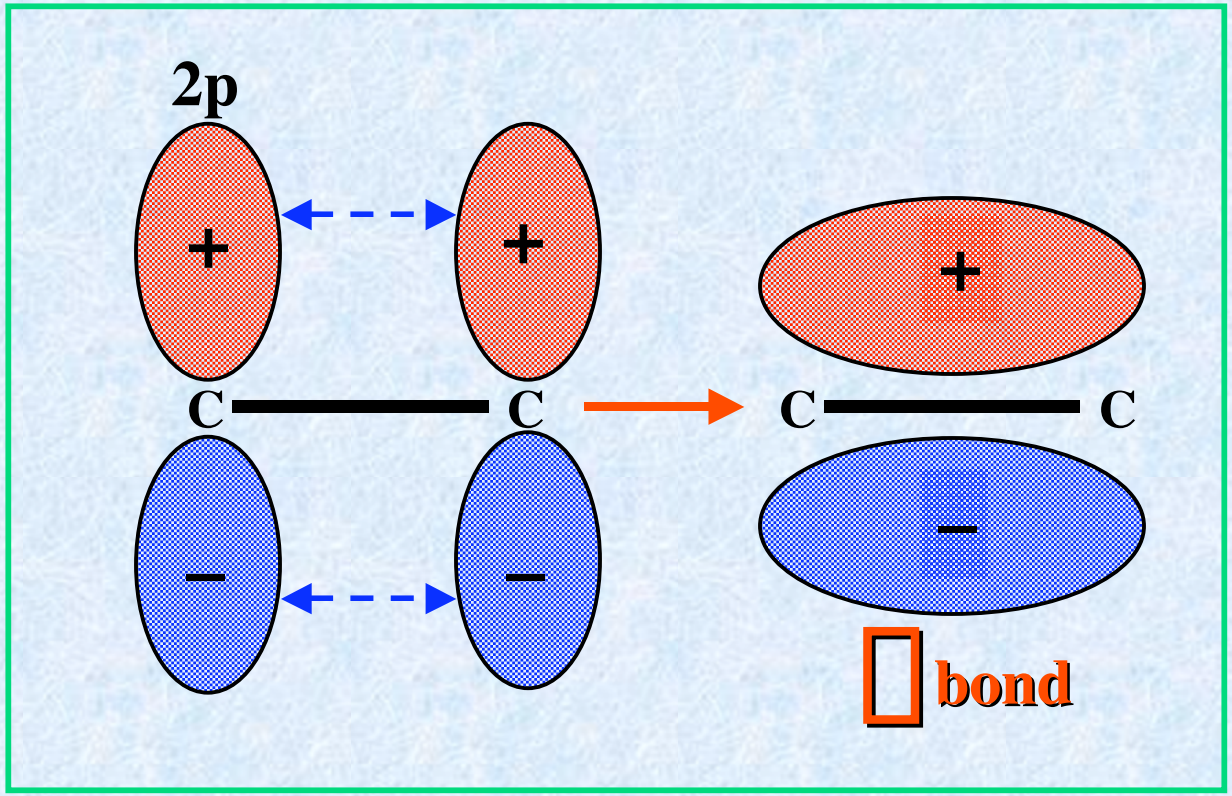
Remaining sp^2 on each c overlap each other gives C-C bond

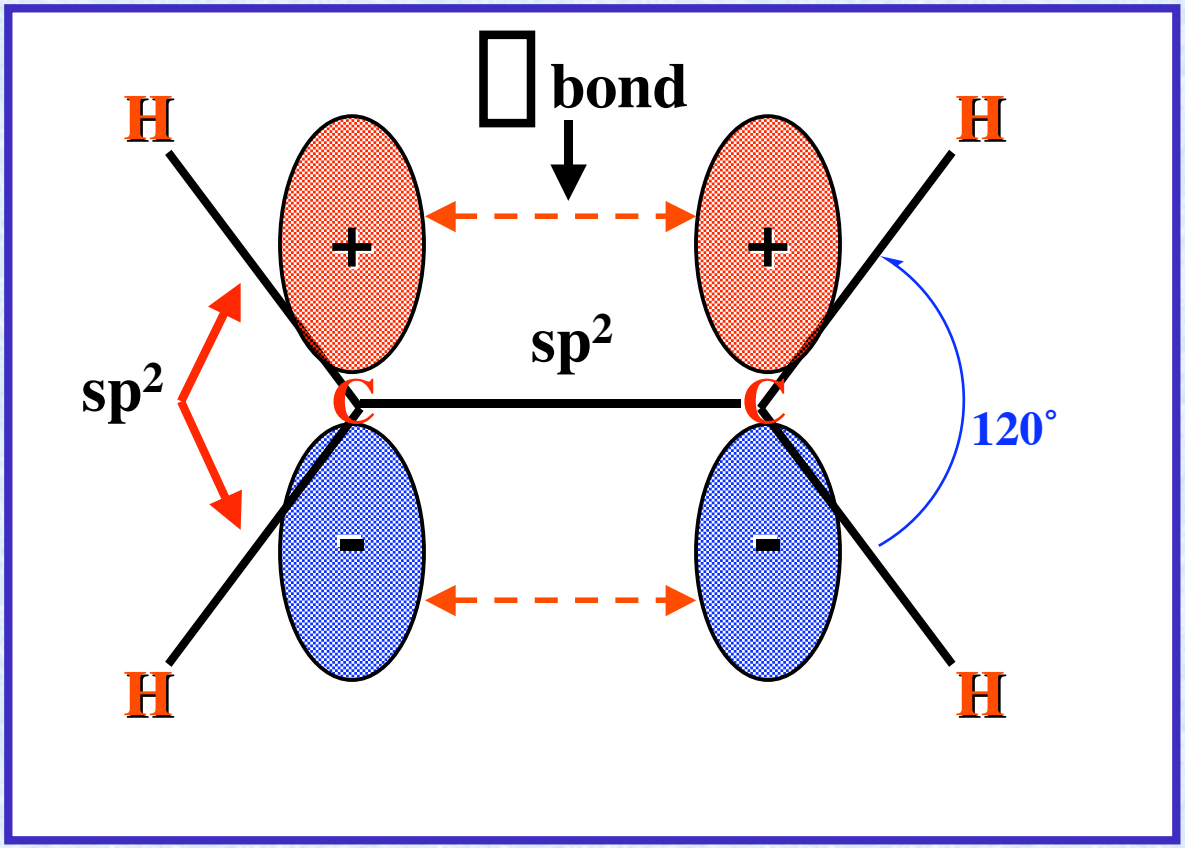
This uses 3 valence e^- from each C to form 5 sp^2 bonds (bonds)

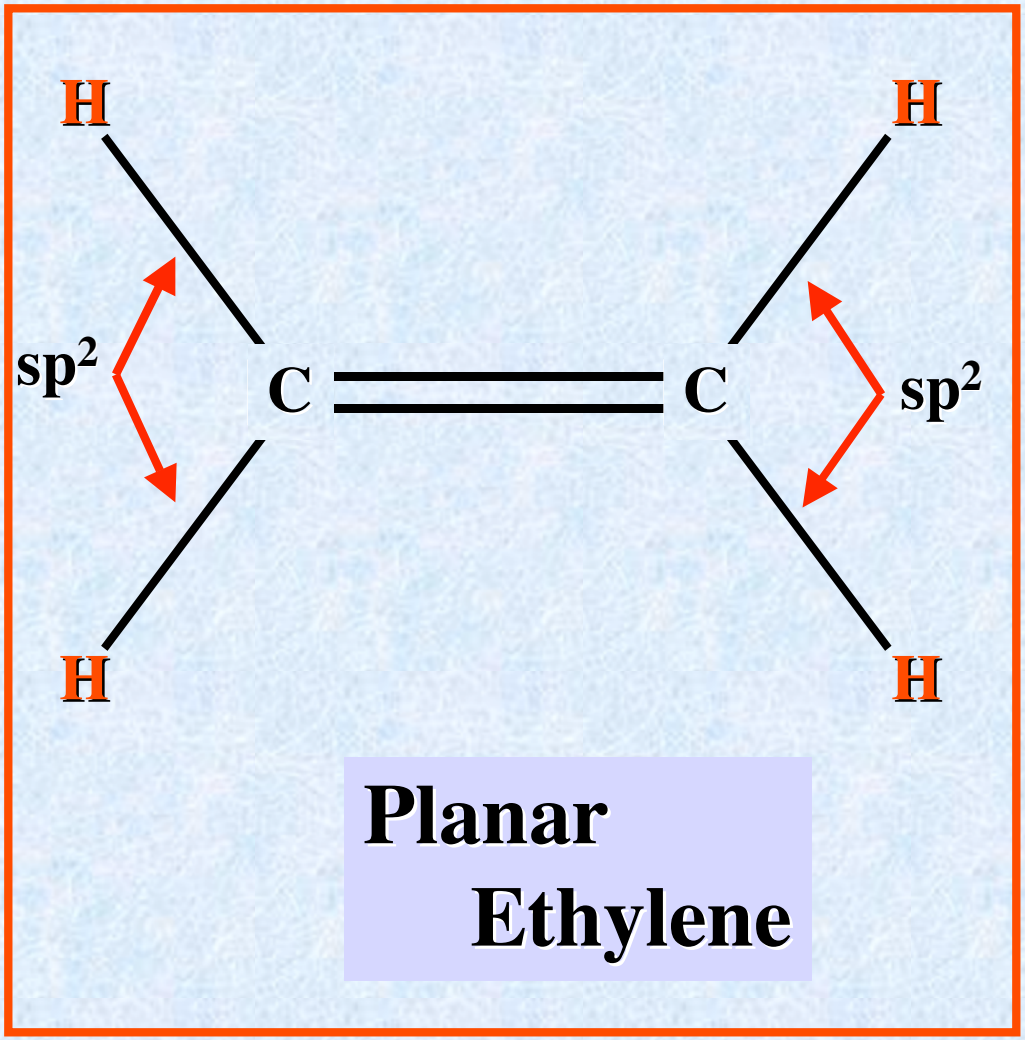


(Each C contributes 1 valence e^- to C-C bond.)

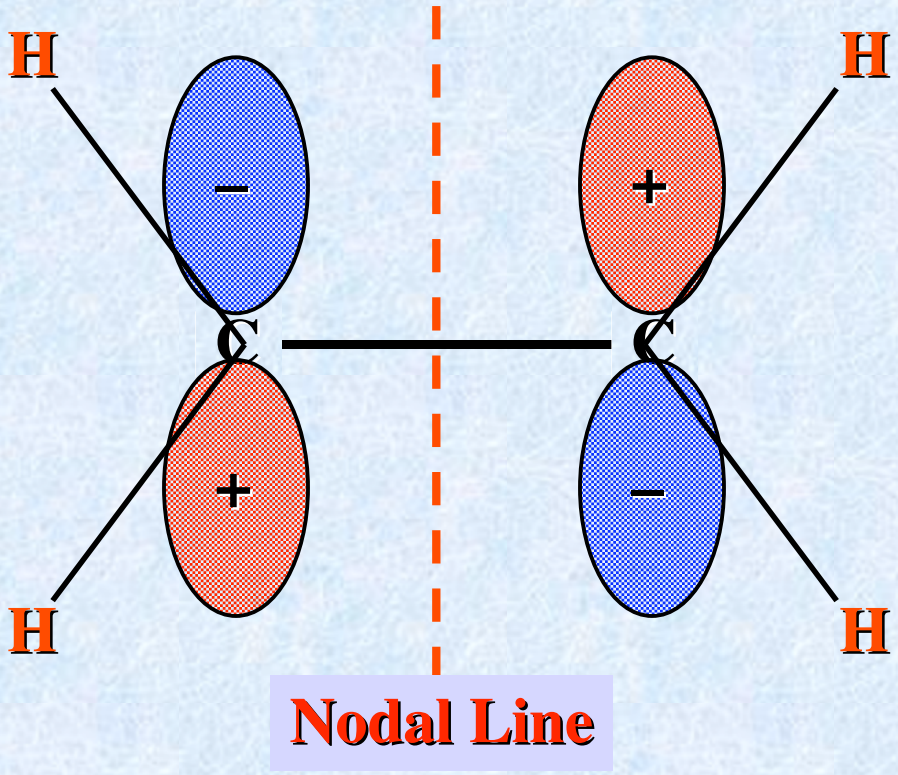
Up to this point, need not be planar because π bond symmetric under rotation.




bond
H
H
+
+
sp2
sp2
C
C
120°
-
-
H
H



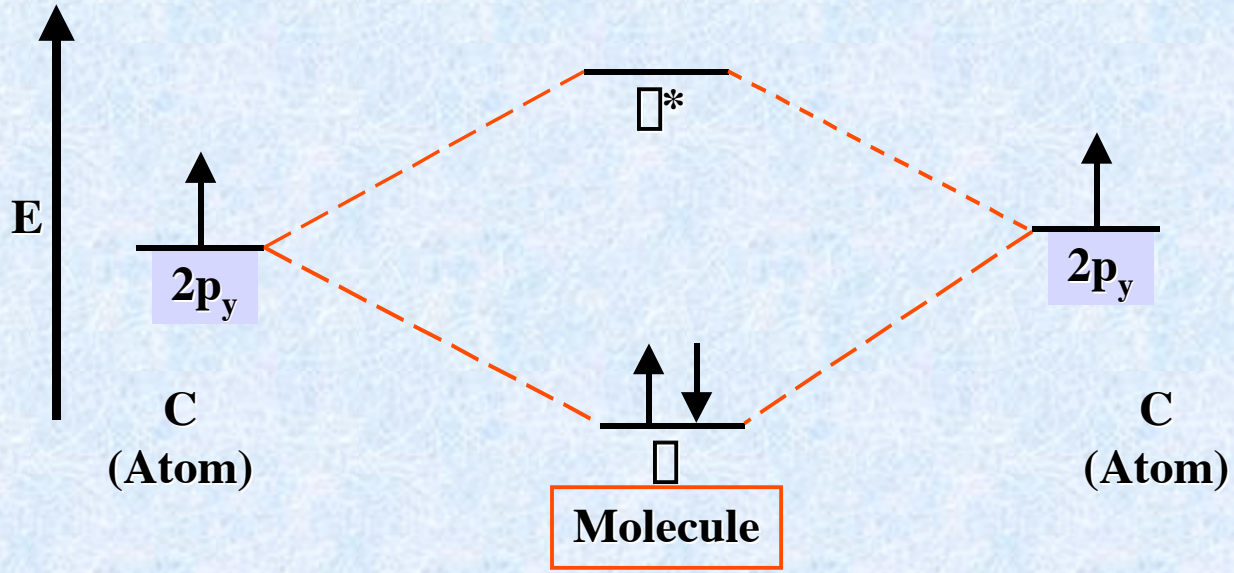
Planar Ethylene



□□ □* transitions in ethylene occur around 1700 Å (58,500 cm^{-1})

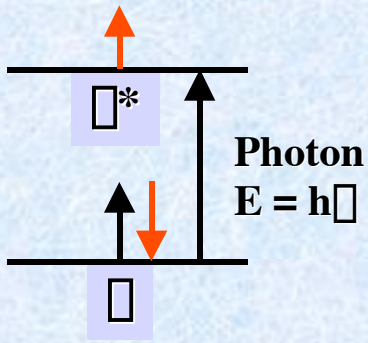
Corresponds to an energy of about 600 kJoules/mole □

□ States in Ethylene



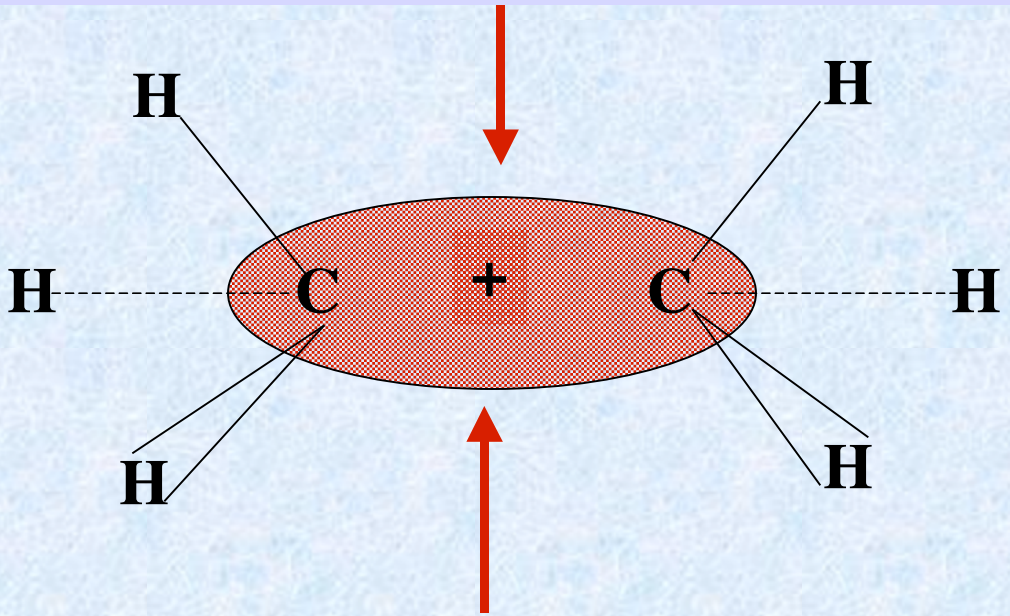
E = h□ = hc/□

□ □1700 Å□



Saturated carbons form only σ bonds, and σ* higher in energy than π* (start to absorb ~ 1600 Å)

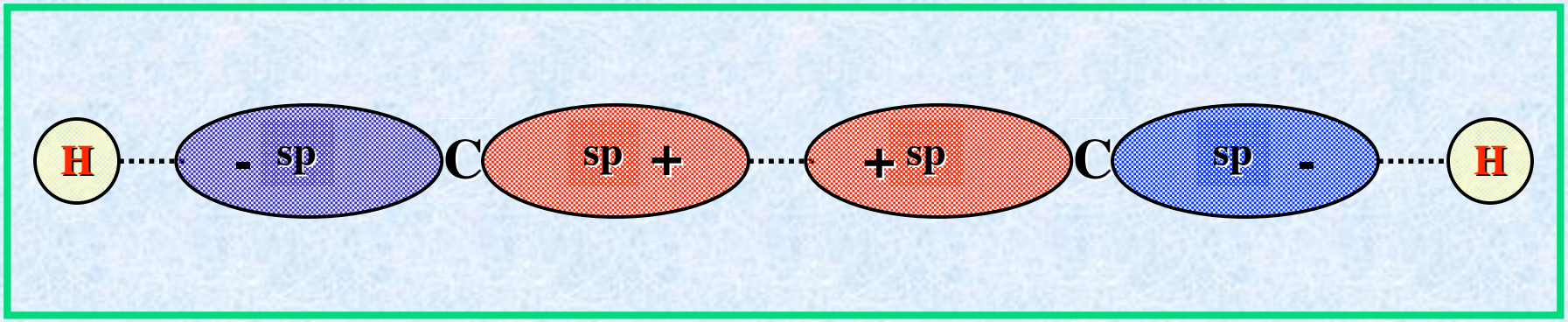
σ bond formed from two sp^3 hybridized orbitals



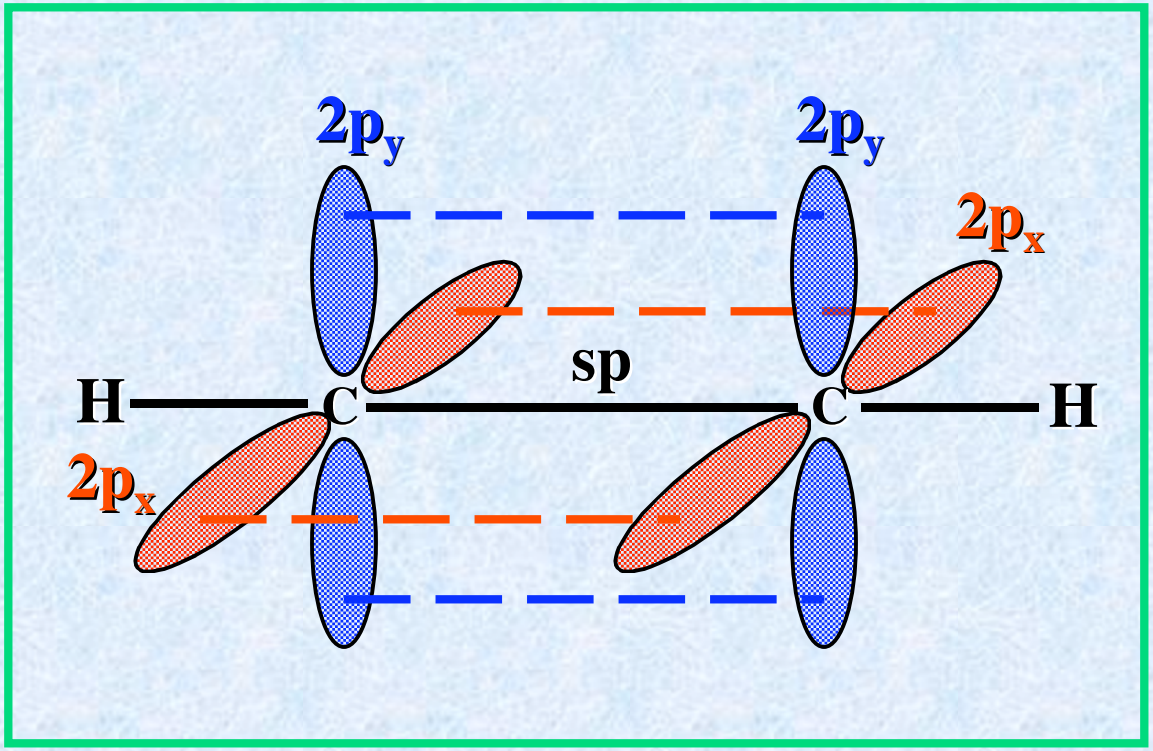
Cylindrically symmetrical about C-C bond.

Carbon sp hybrids: Acetylene and the Triple bond

C_2H_2 is H-CC-H



H-C-C-H

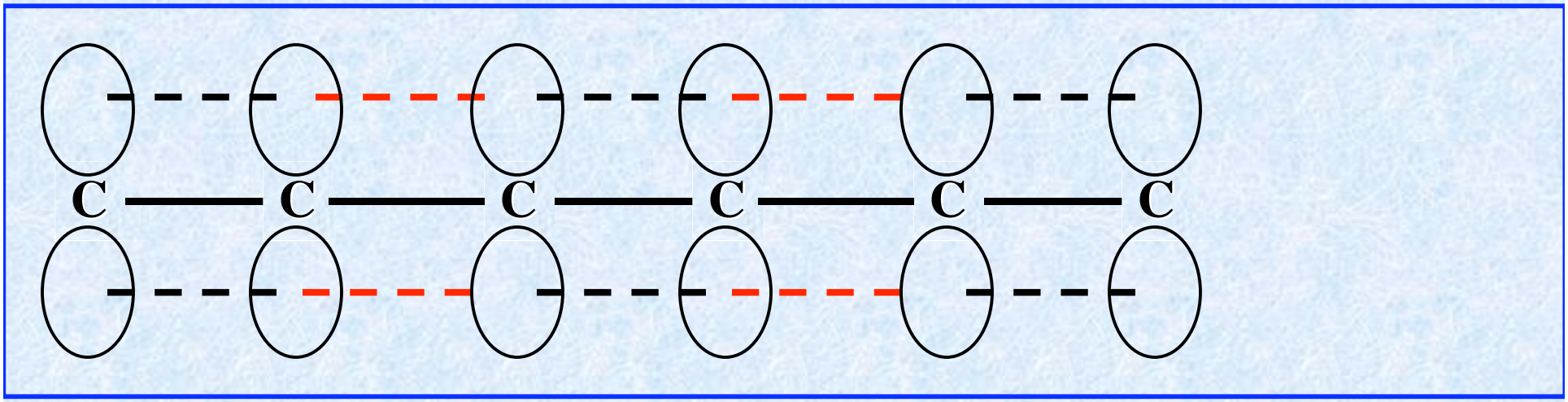


Short Comparison of Bond Order, Bond Length, Bond Energy

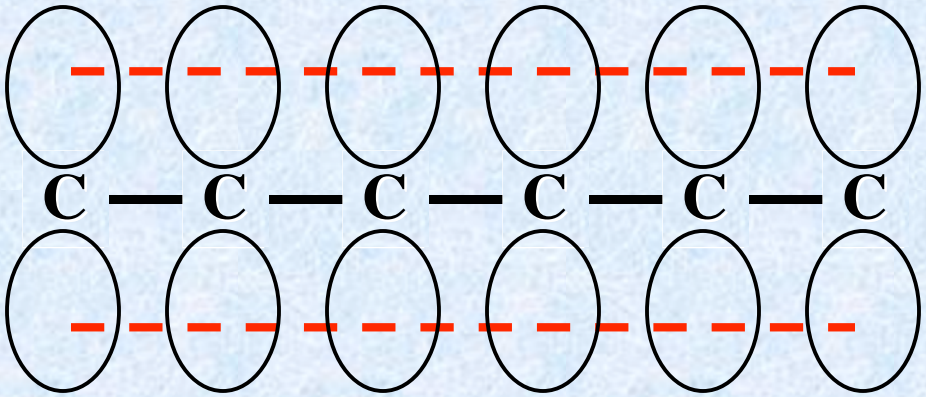
Molecule	C-C Bond Order	C-C Bond Length	C-C Bond E, kcal/mole
Ethane, C_2H_6	1 (1 □)	1.54Å	83
Ethylene, C_2H_4	2 (1□, 1π)	1.35Å	125
Acetylene, C_2H_2	3 (1□, 2π)	1.21Å	230

Although energy of π^* in ethylene < σ^*, conjugated polylenes have even lower energy π^* levels. These absorb light at longer wavelength- sometimes even in visible (human eye's light perception). Conjugated polyenes:

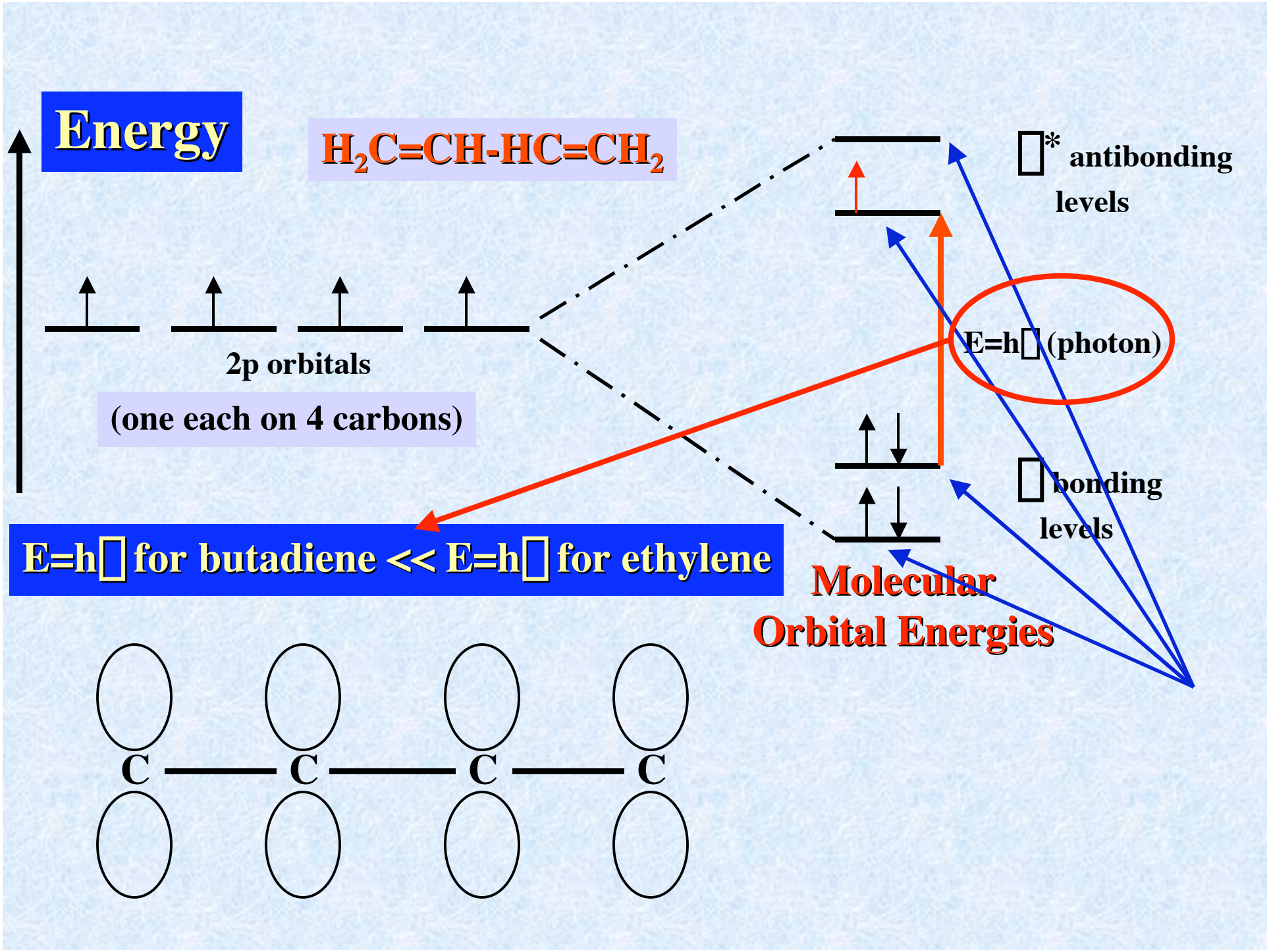
C=C-C=C-C=C polyene

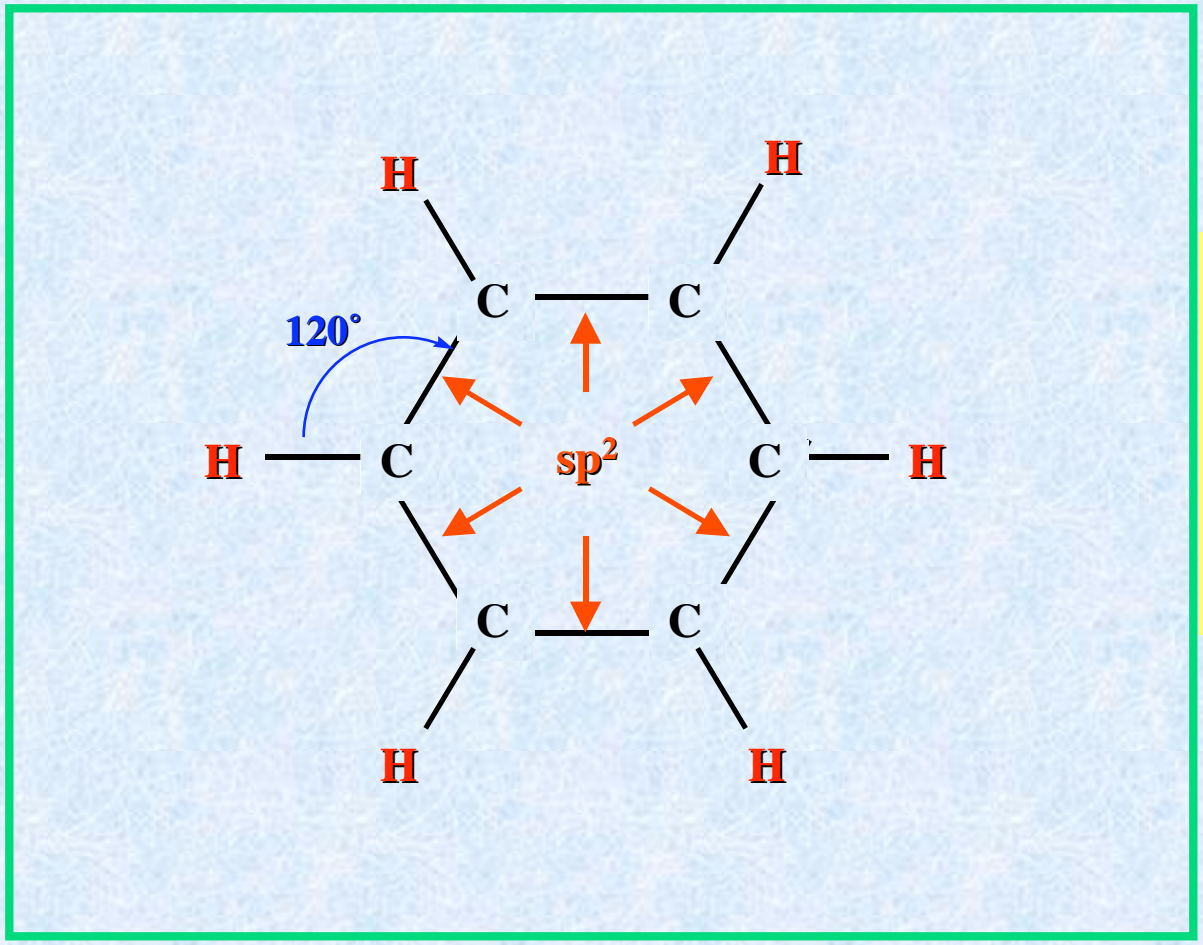


This gives **delocalized** structure

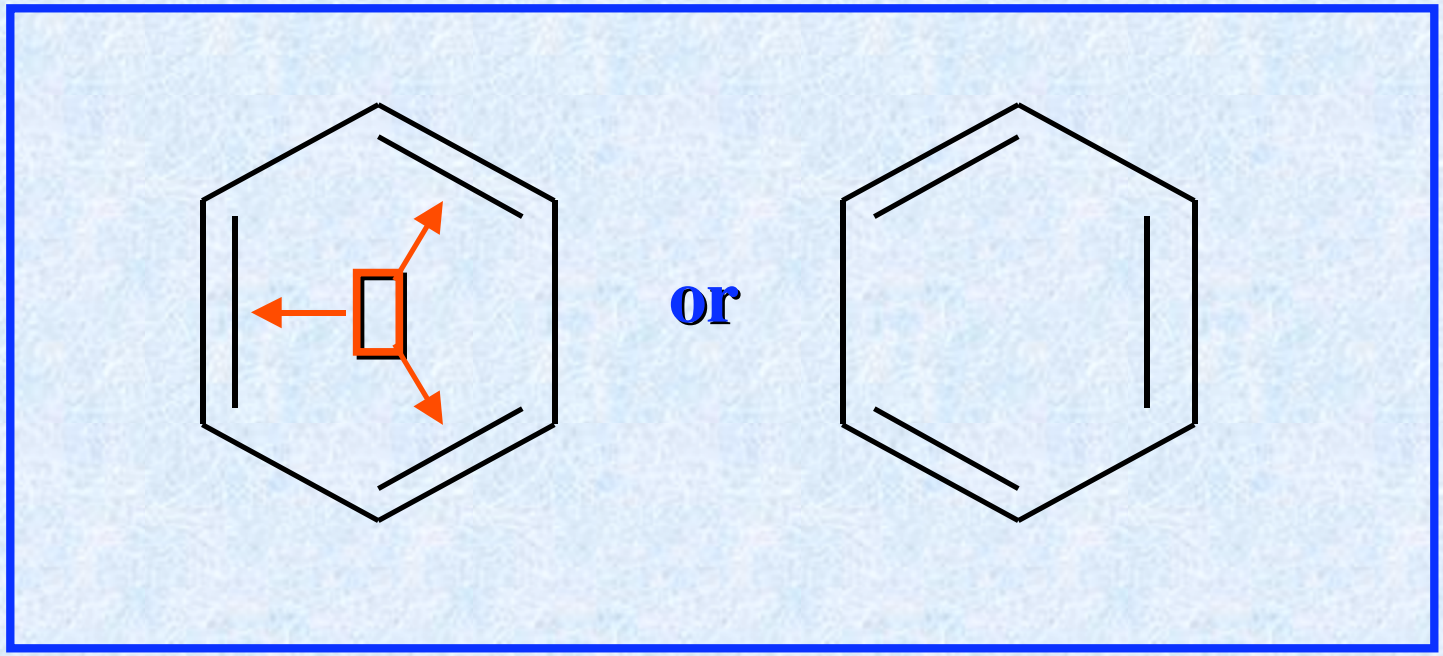


ψ_{MO} = (Const)[$2p_y(1) + 2p_y(2) + 2p_y(3) + 2p_y(4) + 2p_y(5) + 2p_y(6) + \ldots\ldots\ldots$]. Add $2p_y$ Atomic Orbitals on each C


Energy
H2C=CH-HC=CH2
π* antibonding levels
2p orbitals
(one each on 4 carbons)
E=hν (photon)
π bonding levels
E=hν for butadiene << E=hν for ethylene
Molecular Orbital Energies
C
C
C
C

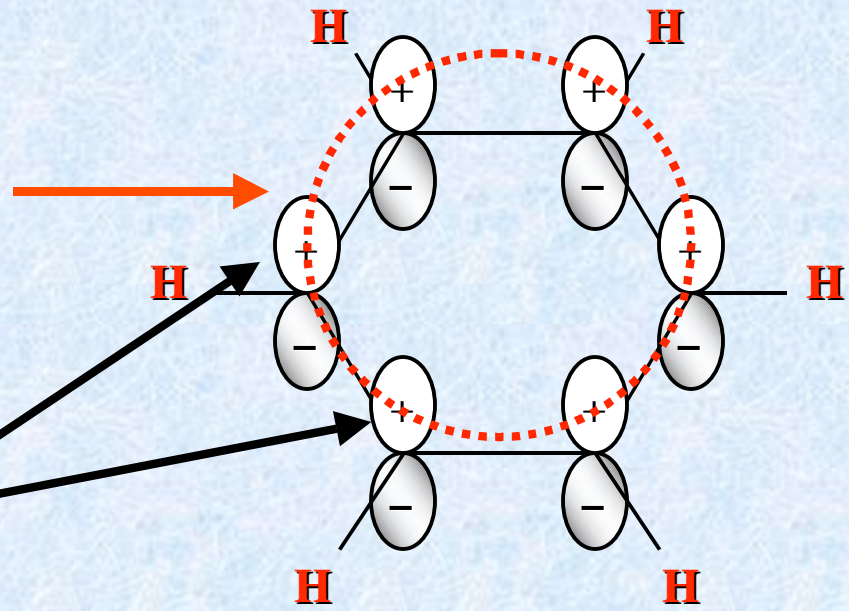


Electron Delocalization in Carbon Ring Compounds



This is **localized** picture!

Delocalized Picture



Can form π bonds with these p orbitals.

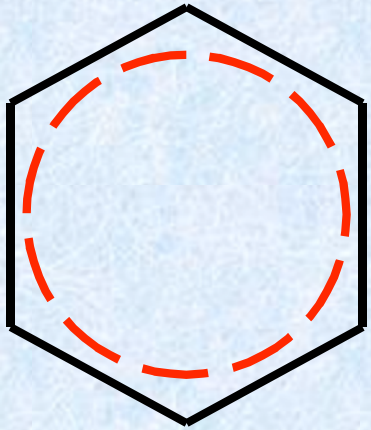
$$\psi_{MO} = (\text{Const})[2p_y(1) + 2p_y(2) + 2p_y(3) + 2p_y(4) + 2p_y(5) + 2p_y(6)]$$

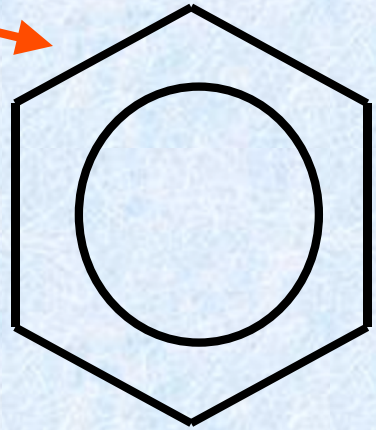
Add 6 $2p_y$ Atomic Orbitals on each C

There are 6 such combinations!

ψ_{MO} = (Const)[$2p_y(1)$ + $2p_y(2)$ + $2p_y(3)$ + $2p_y(4)$ +$2p_y(5)$ + $2p_y(6)$]

Add 6 $2p_y$ Atomic Orbitals on each C





**Can actually form a total of 6 delocalized M.O.'s for benzene (6 2p Atomic Orbital's 6 M.O.'s). **