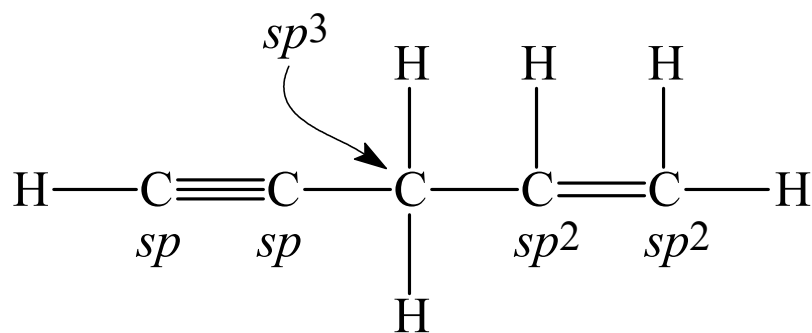


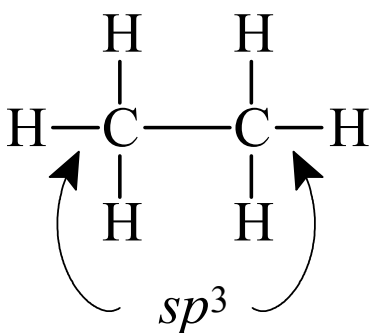
Hybridization and Shape

- L The domain geometry and shape about central atoms in a complex molecule can be rationalized in terms of hybridization.
- L In the VB model, a sigma bond is always assumed to exist between bonded atoms.
- L The directional nature of sigma bonds, often using hybrid orbitals, makes the geometry about a central atom.

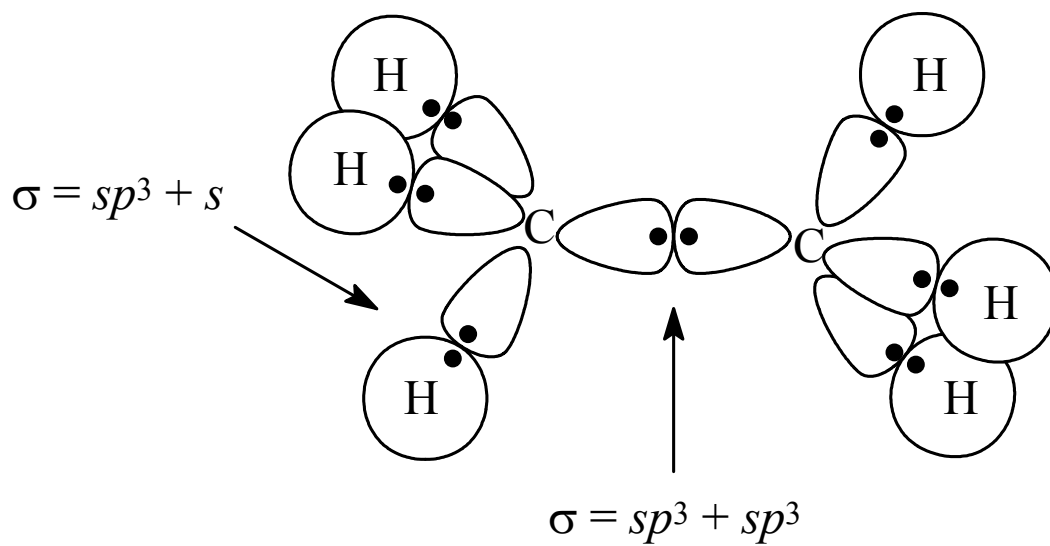


VB Model of Ethane, C_2H_6

Lewis model:



VB model:

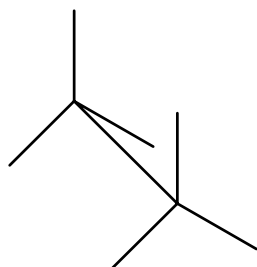


Hindered Rotation in C₂H₆

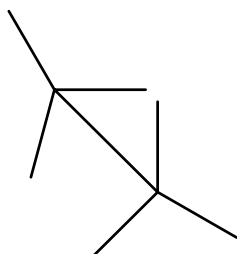
- L Relatively free (slightly hindered) rotation can occur about a single bond axis.
- L Hindered rotation leads to stereochemical conformations in ethane.
 - The barrier to rotation is ~12 kJ/mol in C₂H₆.
 - The various fluxional forms are called *conformers*.

Conformers of Ethane

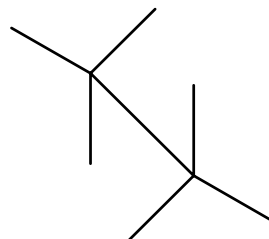
“Sawhorse” Representations of ethane's conformers:



Eclipsed
(highest energy)

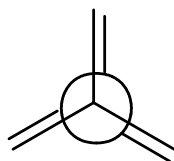


Gauche

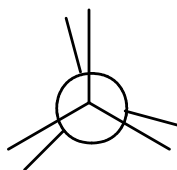


Staggered
(lowest energy)

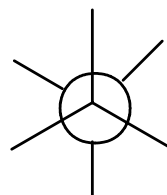
Newman Projections of ethane's conformers:



Eclipsed
(highest energy)



Gauche

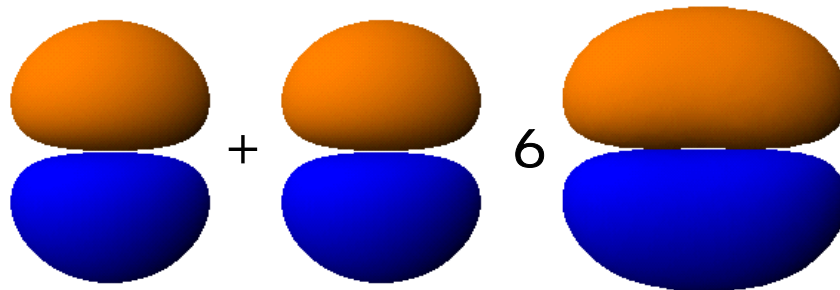


Staggered
(lowest energy)

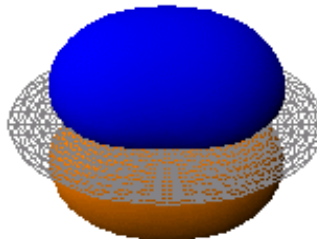
Orbital Overlap in Double and Triple Bonds

Pi Bonding (π bonds)

- L Pi bonding results from side-by-side overlap of two orbitals, such as two $2p_x$ or two $2p_y$ orbitals.



Rotated about bond axis to show nodal plane:

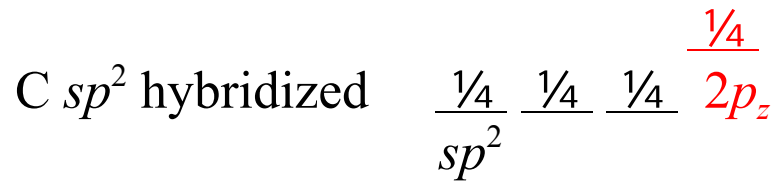
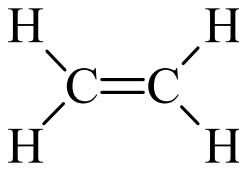


- L In the VB approach, there is never a π bond without a σ bond, too.

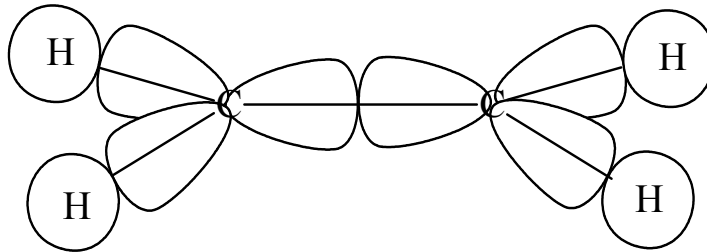
Composition of Bonds by Overlap Type

Bond Type	Composition	Maximum Electron Density
single	σ	along z
double	$\sigma + \pi_x$ or $\sigma + \pi_y$	along z (σ) in xz or yz plane (π_x or π_y)
triple	$\sigma + \pi_x + \pi_y$	along z (σ) in xz plane (π_x) and yz plane (π_y)

Sigma and Pi Bonding in C₂H₄

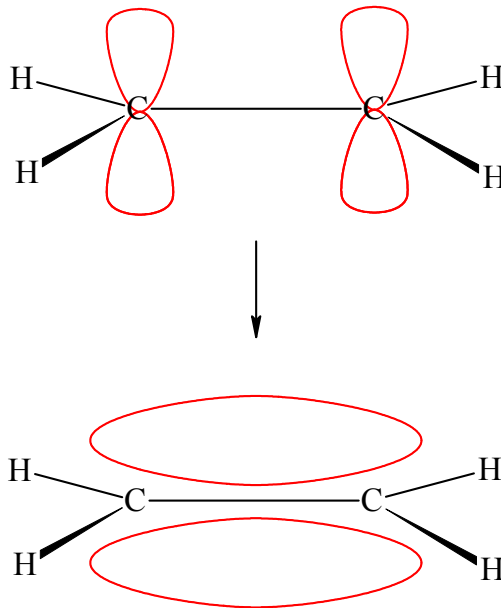


Sigma



Bonding:

Pi Bonding:

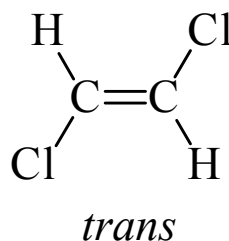
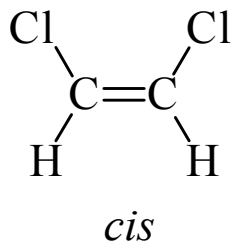


Stereochemical Rigidity and Isomers

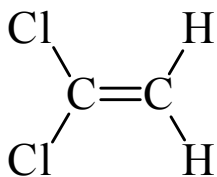
- Rotation is severely restricted about a double bond, creating *stereochemical rigidity* and the possibility of *isomers*.

Isomers – different compounds with the same molecular formula

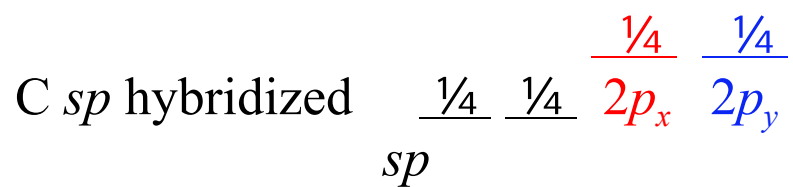
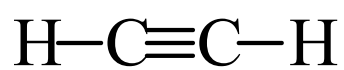
Stereoisomers – isomers that differ only in how their atoms are oriented in space.



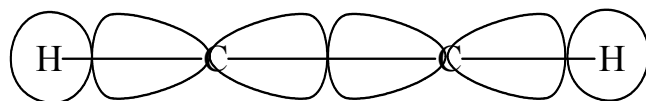
- Cis-trans* isomers are also called **geometrical isomers**, because they differ in the geometry of the atoms or groups of atoms about the double bond.
- Structural isomers** (or **constitutional isomers**) have the same formulas but different atoms bonded together.



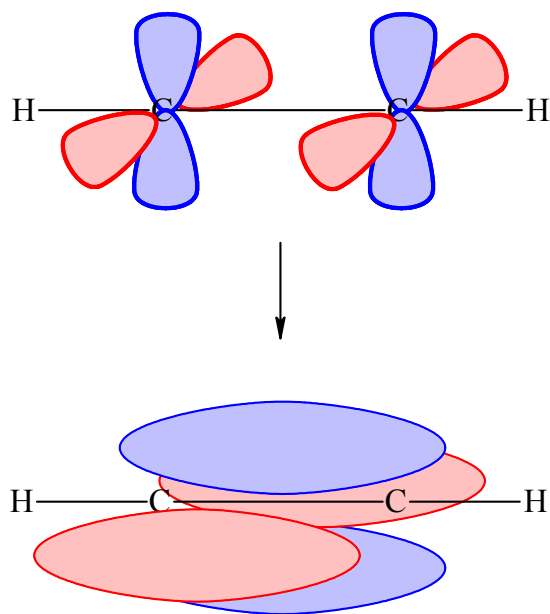
Triple Bond in C₂H₂



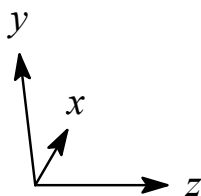
Sigma Bonding:



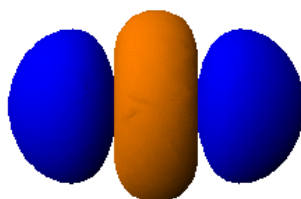
Pi Bonding:



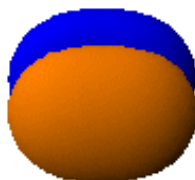
Boundary Surface Models of the Sigma and Two Pi Bonds in C₂H₂



$\sigma(z)$



$\pi(xz)$



$\pi(yz)$

