Quantum Mechanics and Bonding Hybridization

Chapter 4.6

How are Bonds Formed?

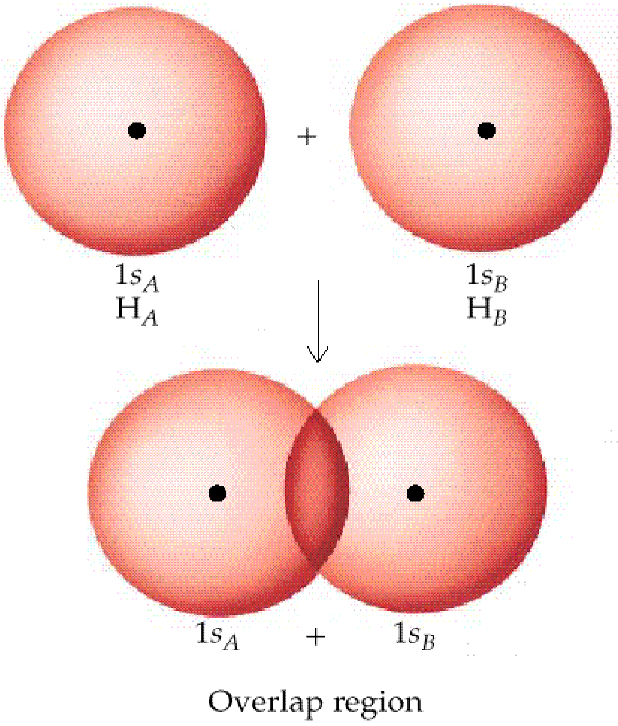
- THE STORY SO FAR…
  - The **Lewis structure** of a molecule provides a simplified view of *bond formation* and allows us to determine the *number of bonding and lone electron pairs*
  - **VSEPR theory** can then be used to predict the *molecular geometry*
  - We can even use **electronegativity values** to determine *bond polarity* and **bond dipoles** to determine the overall *molecular polarity*
- BUT…
  - Lewis structures, VSEPR theory, and bond dipoles do not describe *how bonds are actually formed*

Valence Bond Theory

- **Valence bond theory** is a theory stating that atomic orbitals overlap to form a new orbital with a pair of opposite spin electrons
  - A covalent bond forms when 2 atomic orbitals, each with an unpaired electron, overlap
  - When the covalent bond forms, the lowest energy state is obtained when participating electrons are of opposite spin

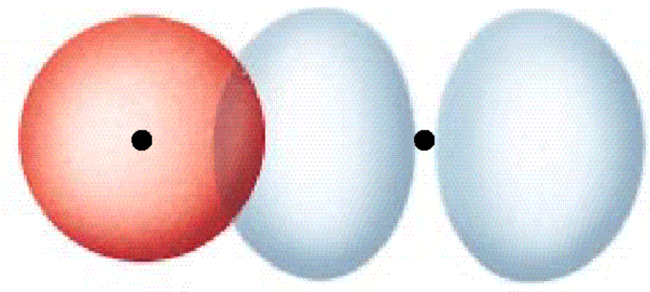
Orbital Overlap

- The covalent bond in hydrogen gas (H_2) is formed when the 1s orbital of one hydrogen atom overlaps with the 1s orbital of another hydrogen atom

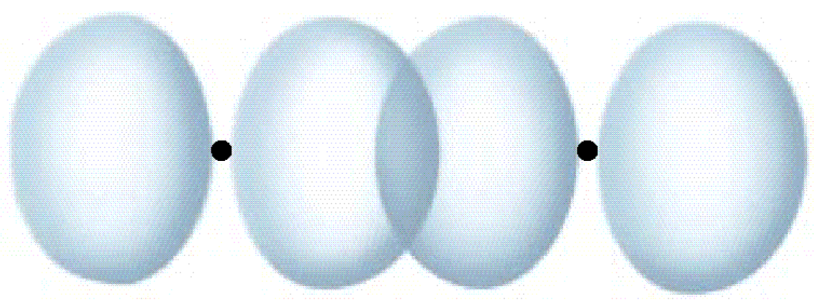


Orbital Overlap

- The covalent bond in HF is formed when hydrogen's 1s orbital and one of fluorine's 2p orbitals overlap

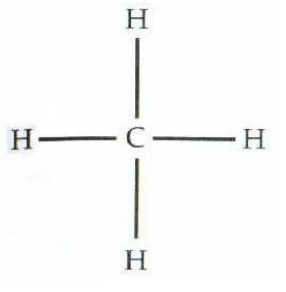


- The covalent bond in F_2 is formed when one of fluorine's 2p orbitals overlaps with one of the 2p orbitals in another fluorine atom



Valence Bond Theory

- Okay, great! Let's use Valence Bond Theory to explain how the orbitals overlap in a methane molecule

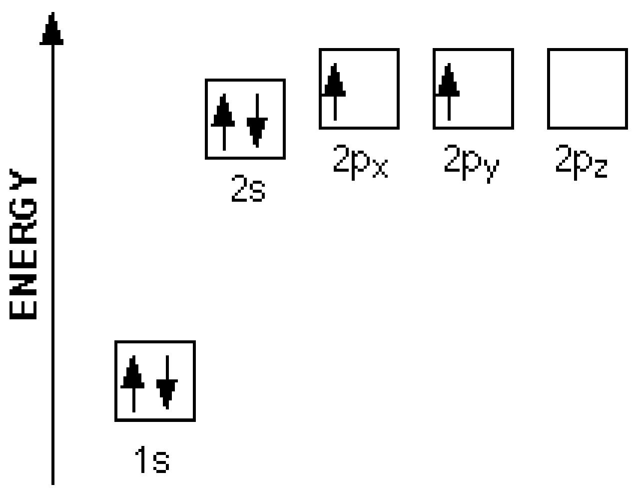


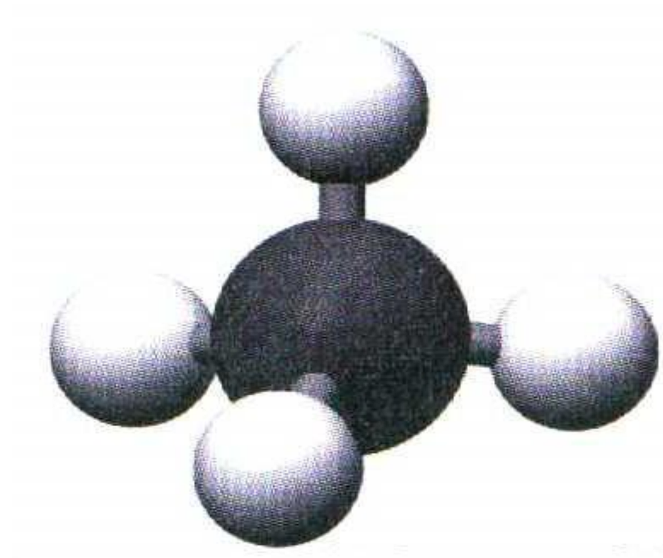
Problem #1

Carbon has only **TWO** orbitals available for overlap

BUT

methane has **FOUR** covalent bonds



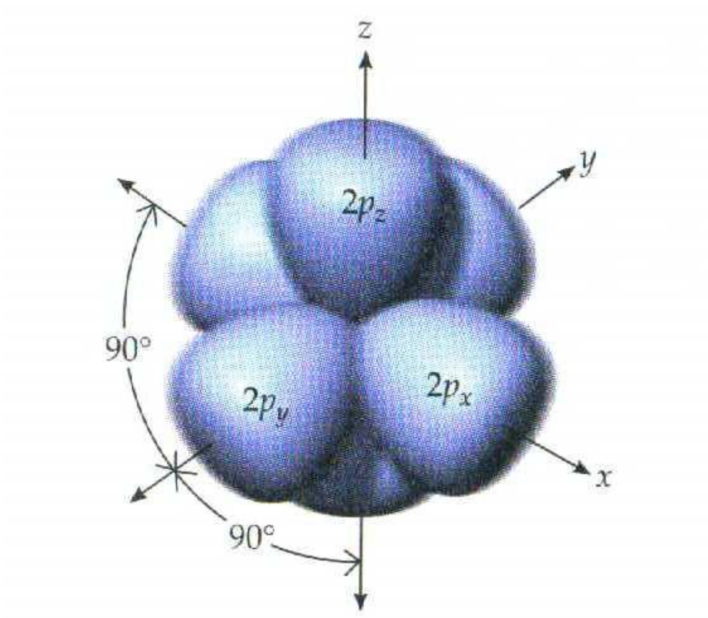


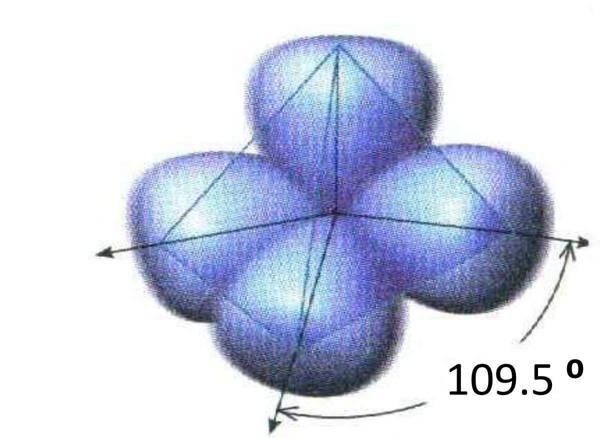
Problem #2

The available p orbitals are at **90º** to one another

BUT

The shape of methane is *tetrahedral* with **109.5º** between bonds





Hybrid Orbitals

- A **hybrid orbital** is an orbital that forms from the combination of at least two different orbitals on an atom
- **Hybridization** is the process of forming hybrid orbitals

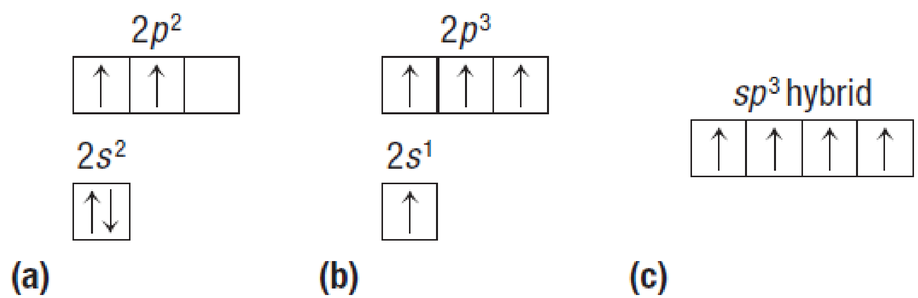
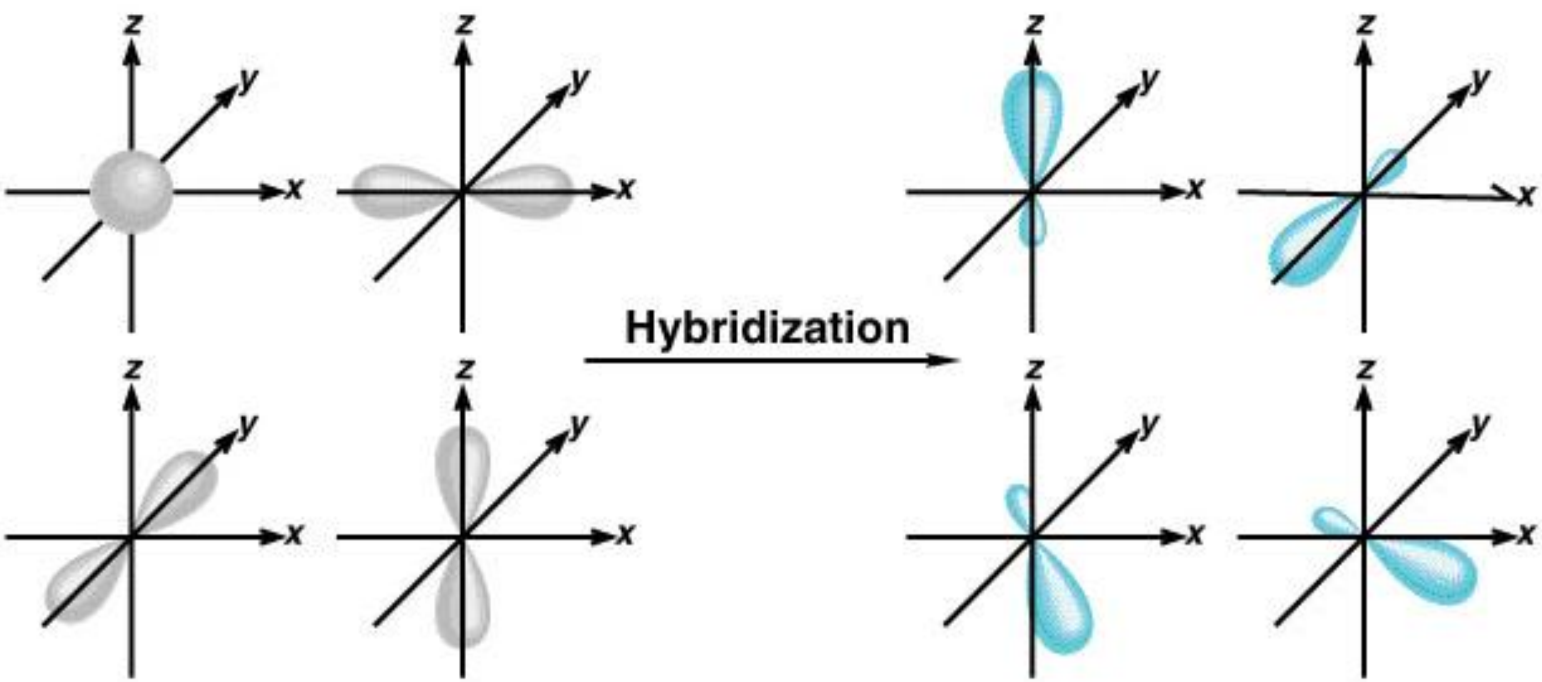


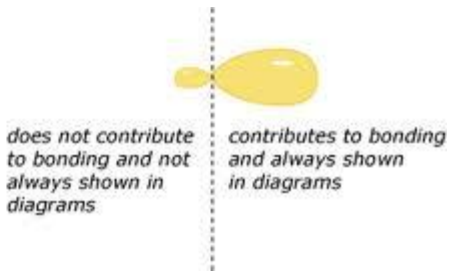
Figure 6 The electrons in a hybrid orbital. (a) A carbon atom with 4 valence electrons has two paired 2*s* electrons and two unpaired 2*p* electrons. (b) To create equal orbitals, a paired electron from the *s* orbital is promoted to the unfilled 2*p* orbital. (c) The *s* and *p* orbitals then merge to form a set of equivalent hybrid sp^3 orbitals, each with 1 unpaired electron. Since four orbitals are combined, four orbitals are produced.

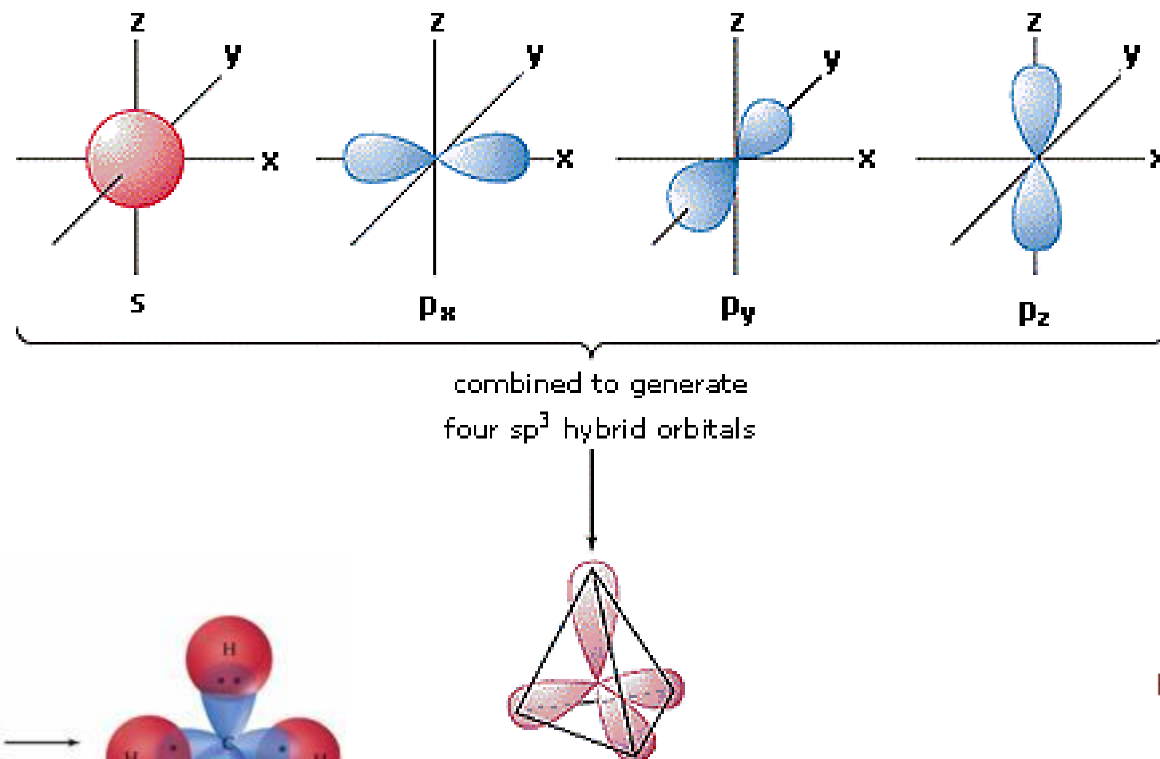
Hybrid Orbitals

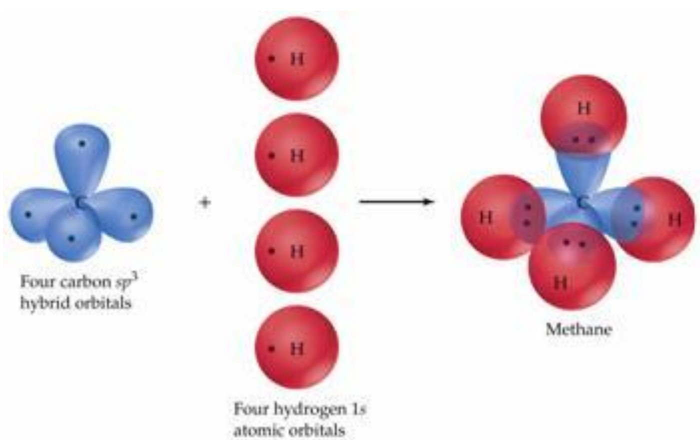
Formation of *sp*^{3} Hybrid Orbitals



sp^3 Hybrid Orbitals







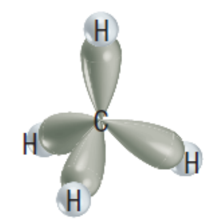
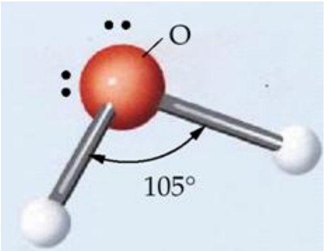
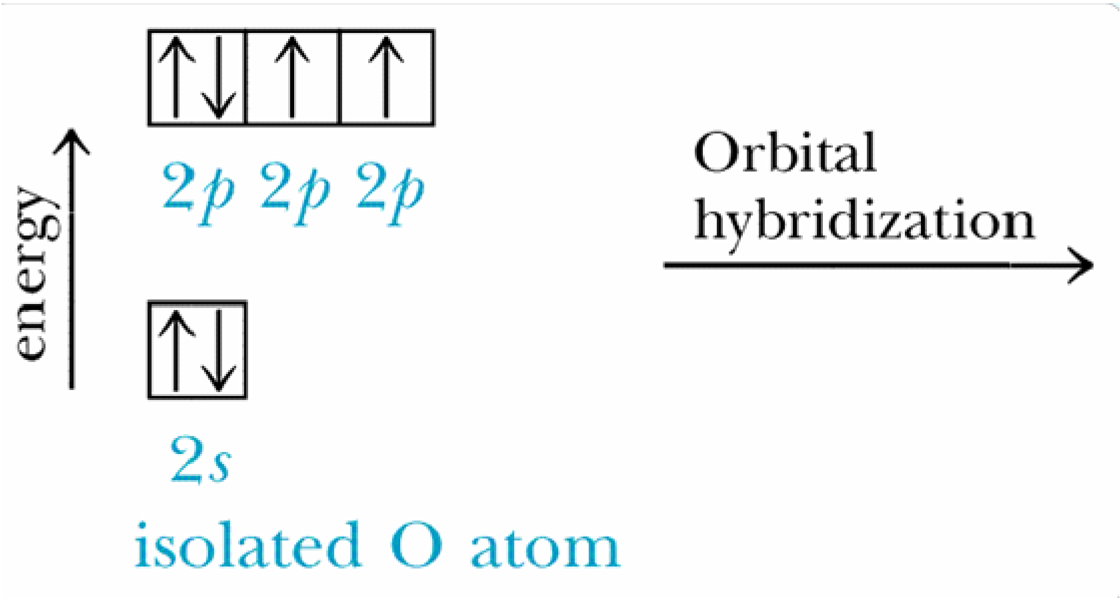
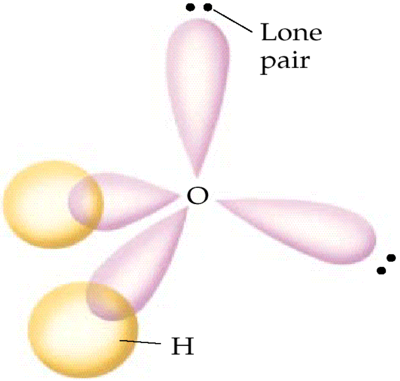


Figure 7 Each bond in a methane molecule arises from the formation of a hybrid sp^3 orbital in the carbon atom. This creates 4 hybrid orbitals with similar properties and results in equivalent chemical bonds with each hydrogen atom.

Let's try it for WATER:

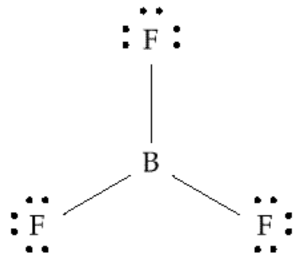




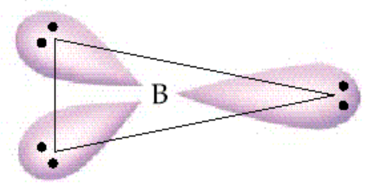


sp^2 Hybrid Orbitals

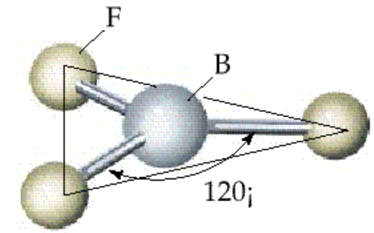
- BF_3 is **trigonal planar** according to VSEPR theory
- we need **3 hybrid orbitals**, so 3 atomic orbitals are required
- s + p + p = **sp^2**



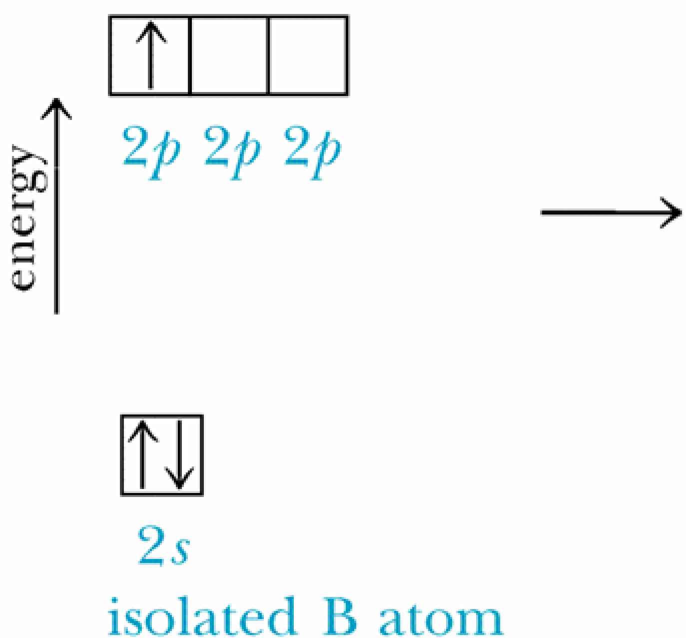
Lewis dot structure



Electron-pair geometry

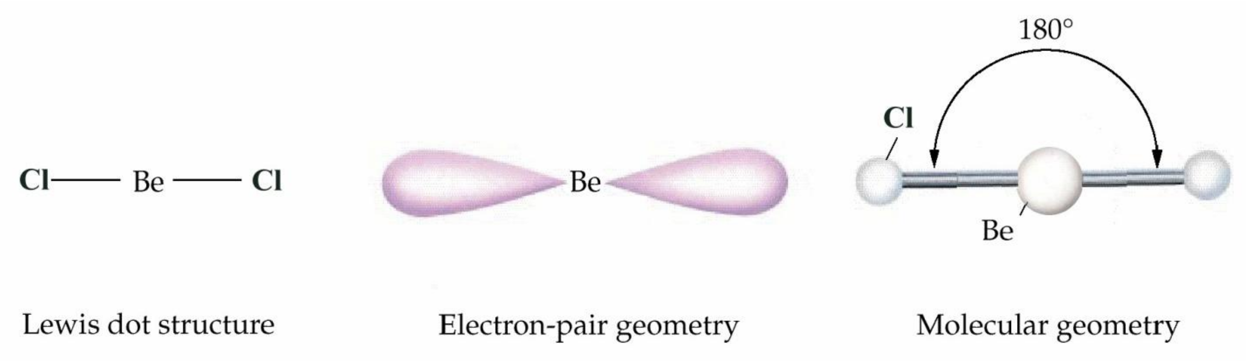


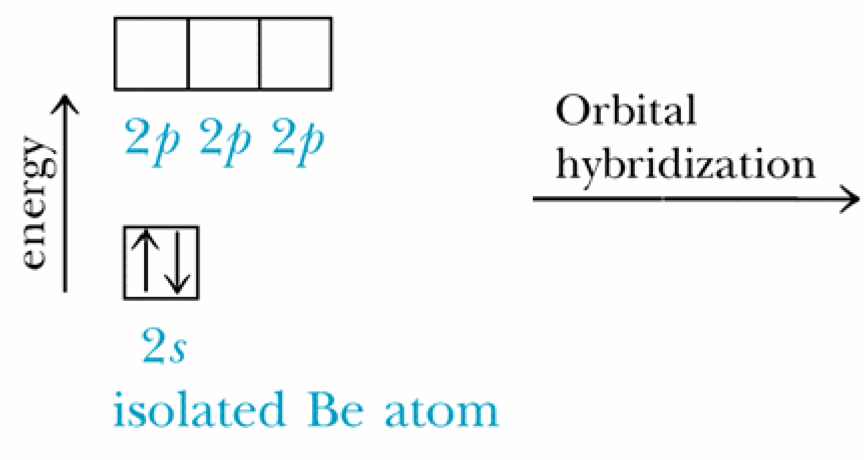
Molecular geometry



sp Hybrid Orbitals

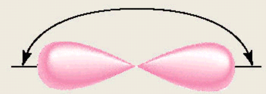
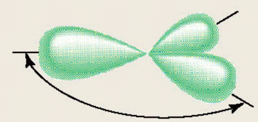
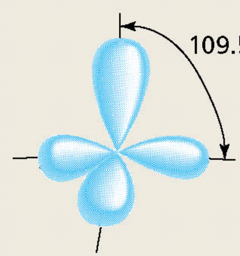
- $BeCl_2$ is **linear** according to VSEPR theory
- we need **2 hybrid orbitals**, so 2 atomic orbitals are required
- s + p = **sp**





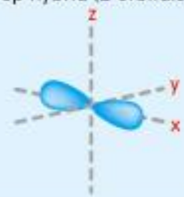
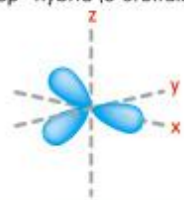
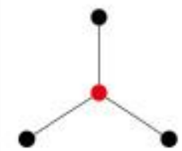
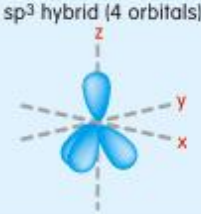
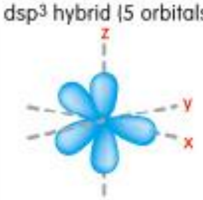
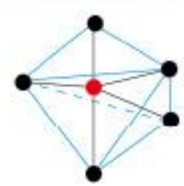
Hybrid Orbitals Summary

Table 10.4 **Important Hybrid Orbitals and Their Shapes**

Pure Atomic Orbitals of the Central Atom	Hybridization of the Central Atom	Number of Hybrid Orbitals	Shape of Hybrid Orbitals	Examples
s, p	*sp*	2	 180° Linear	$BeCl_2$
s, p, p	sp^2	3	 120° Planar	BF_3
s, p, p, p	sp^3	4	 109.5° Tetrahedral	CH_4, NH_4^+

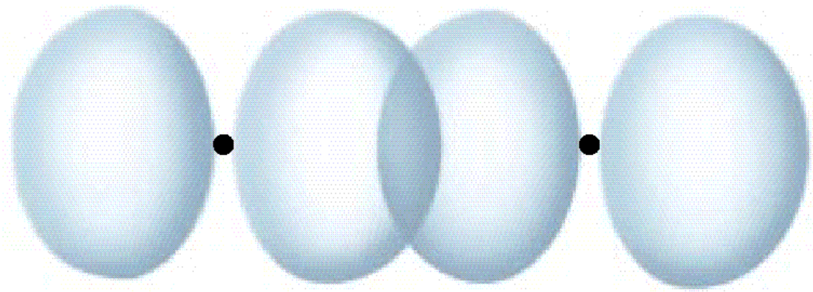
Practice

- Determine the hybrid atomic orbitals that describe the bonding in ammonia

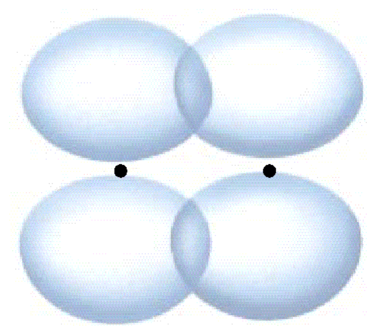
Atomic orbitals combined	Hybrid orbitals formed	Bonding electron pairs and lone pairs around central atom	VSEPR geometry
1 *s* orbital & **1** *p* orbital	sp hybrid (2 orbitals) 	2	 linear
1 *s* orbital & **2** *p* orbitals	sp² hybrid (3 orbitals) 	3	 trigonal planar
1 *s* orbital & **3** *p* orbitals	sp³ hybrid (4 orbitals) 	4	 tetrahedral
1 s orbital & **3** *p* orbitals & **1** *d* orbital	dsp³ hybrid (5 orbitals) 	5	 trigonal bipyramidal
1 s orbital & **3** *p* orbitals & **2** *d* orbitals	d²sp³ hybrid (6 orbitals) 	6	 octahedral

Sigma and Pi Bonds

- A **sigma bond** is formed when the lobes of two orbitals overlap end to end (electron density is between the nuclei, along the internuclear axis)

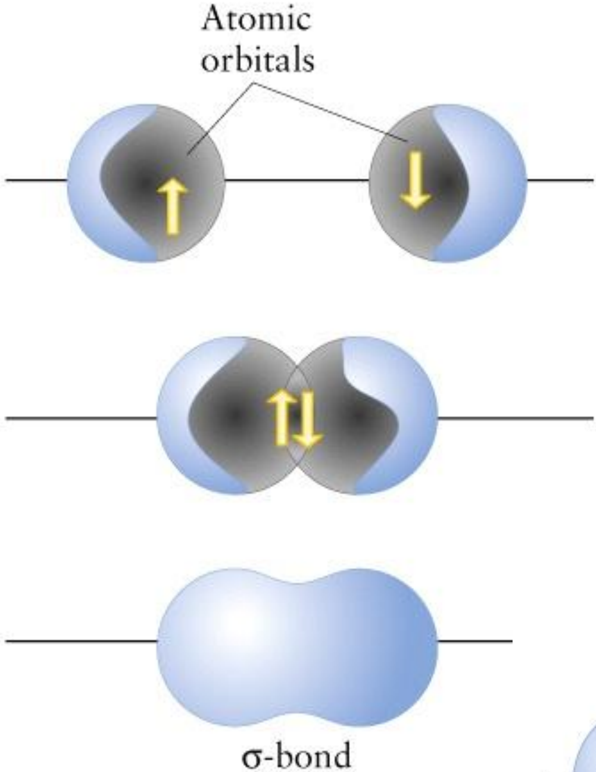


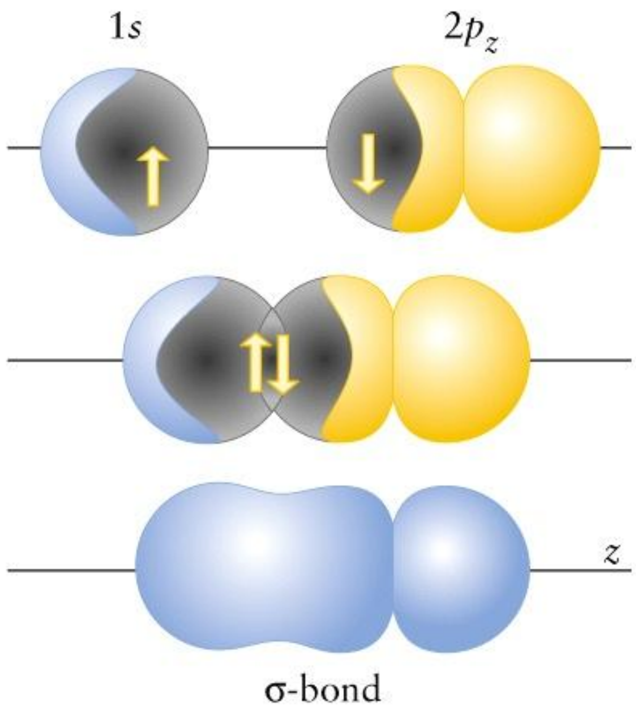
- A **pi bond** is formed when the lobes of two orbitals overlap side by side (electron density is above and below (or in front of and behind) the internuclear axis

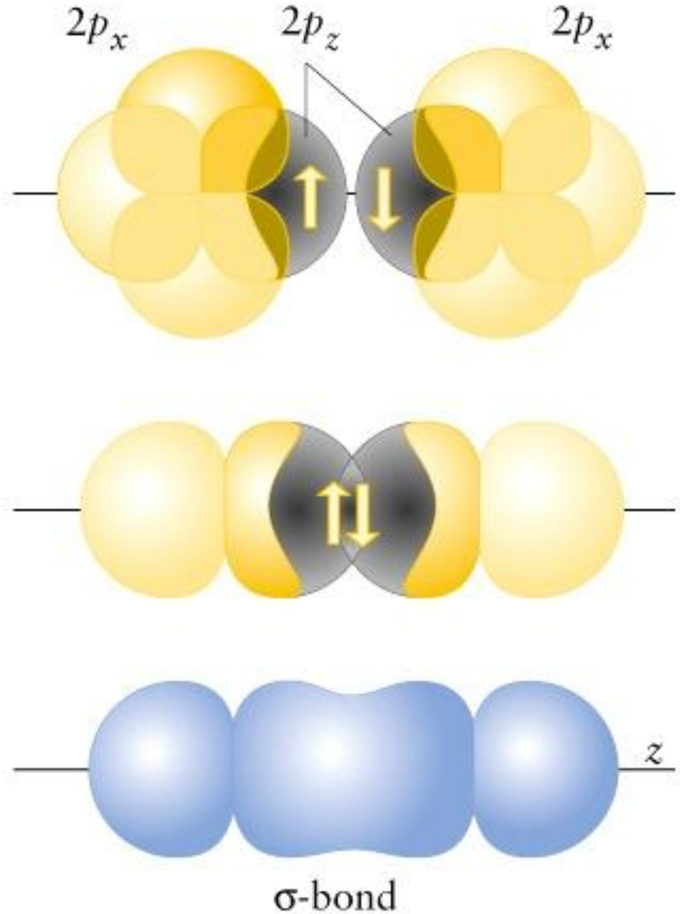


π bond

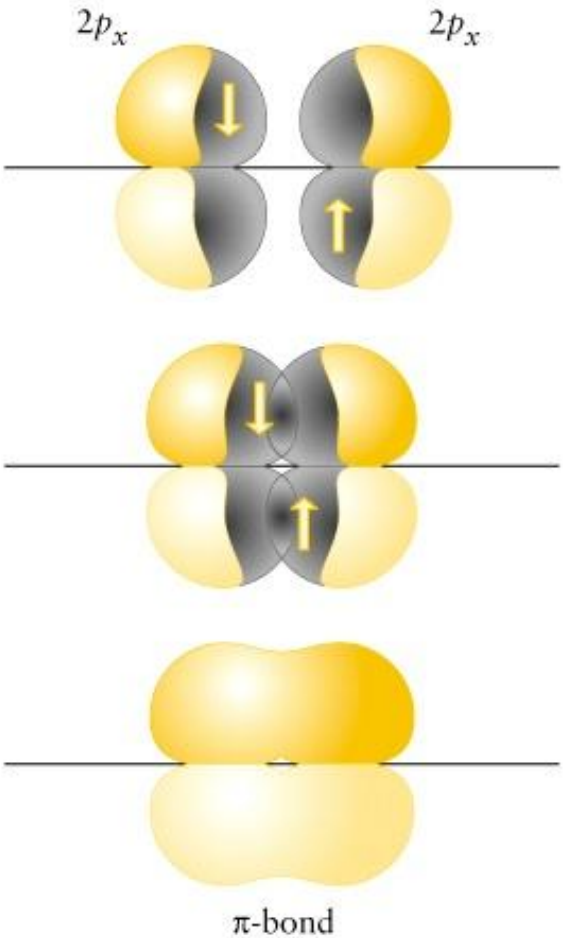
Sigma Bonds

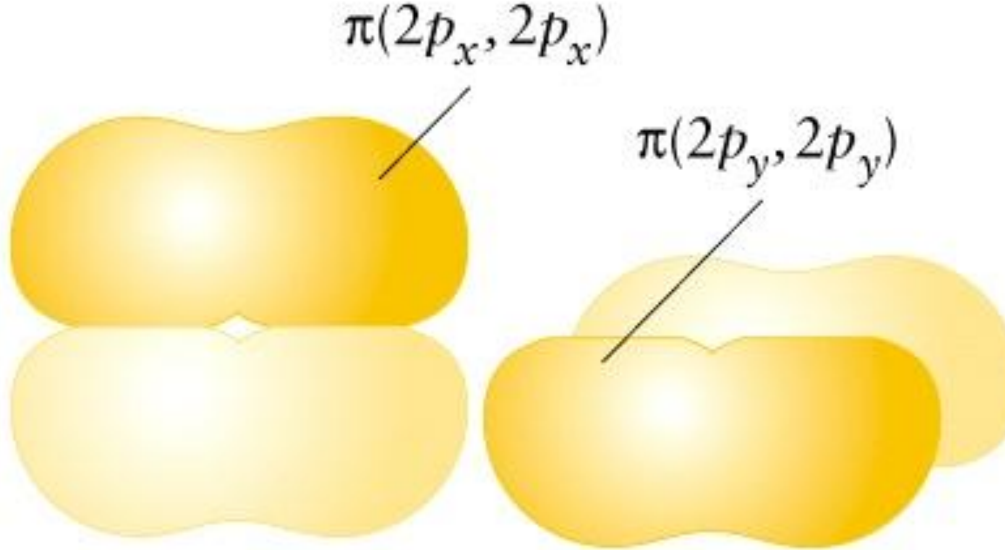






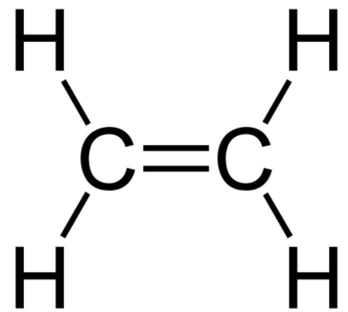
Pi Bonds





Double Bonds

Consider the molecule **ethene**:



What **VSEPR shape** should the central atoms have?

What type of **hybrid orbitals** should the central atoms have?

Double Bonds

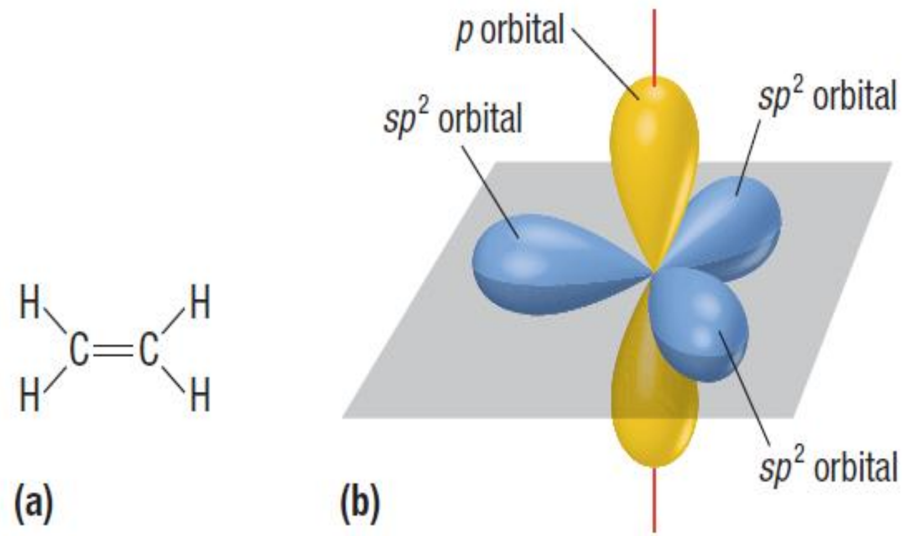
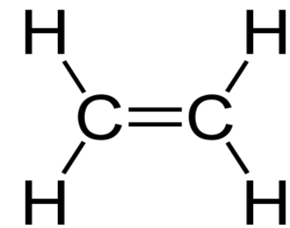
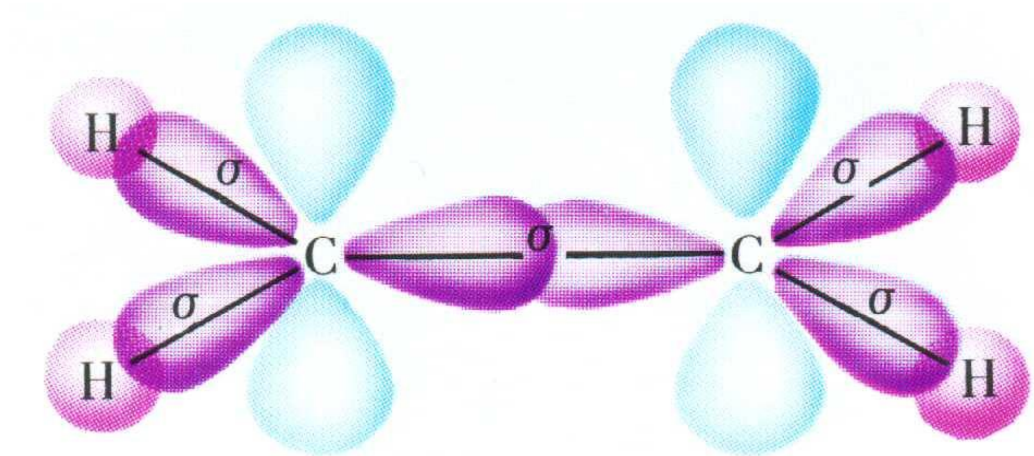


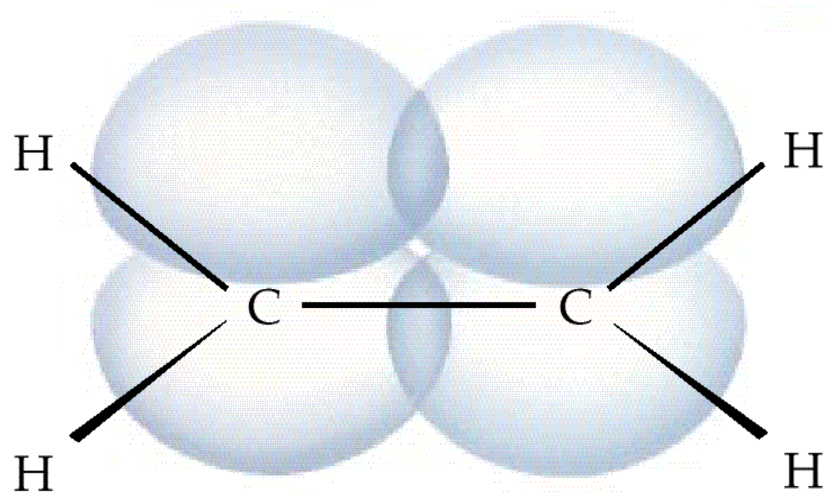
Figure 12 (a) Structural formula of ethene, C_2H_4. (b) In the ethene molecule, an *s* and a *p* orbital hybridize to form three sp^2 orbitals. A single *p* orbital remains perpendicular to the plane of the hybrid orbitals.

Double Bonds

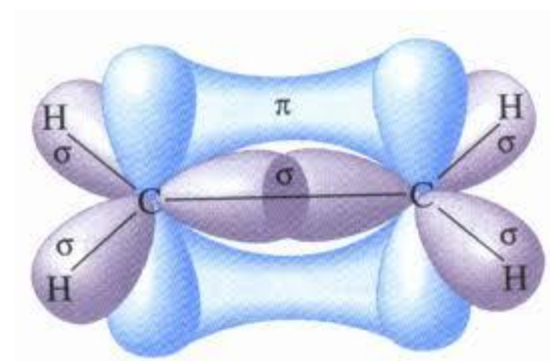




Sigma bonds form between:
•the sp^2 orbital of one carbon with the sp^2 orbital of the other carbon
•The sp^2 orbital of carbon and the s orbital of each hydrogen



Pi bonds form between:
•The p orbitals of the two carbon atoms



Triple Bonds

Consider the molecule **ethyne**:

What **VSEPR shape** should the central atoms have?

What type of **hybrid orbitals** should the central atoms have?

Triple Bonds

$H-C\equiv C-H$

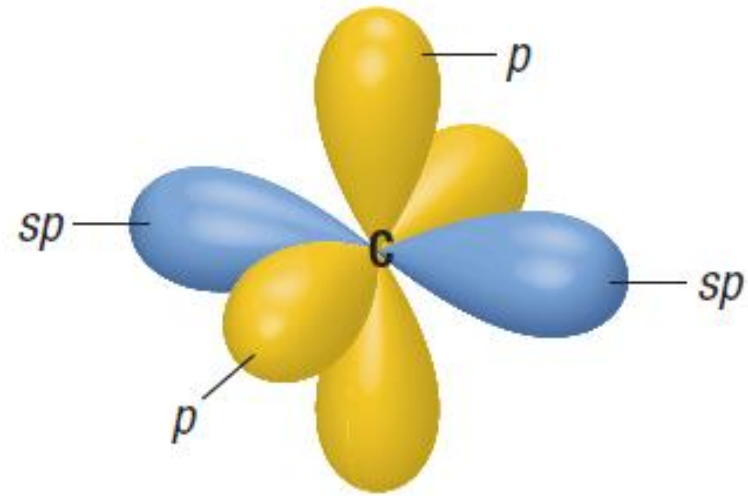
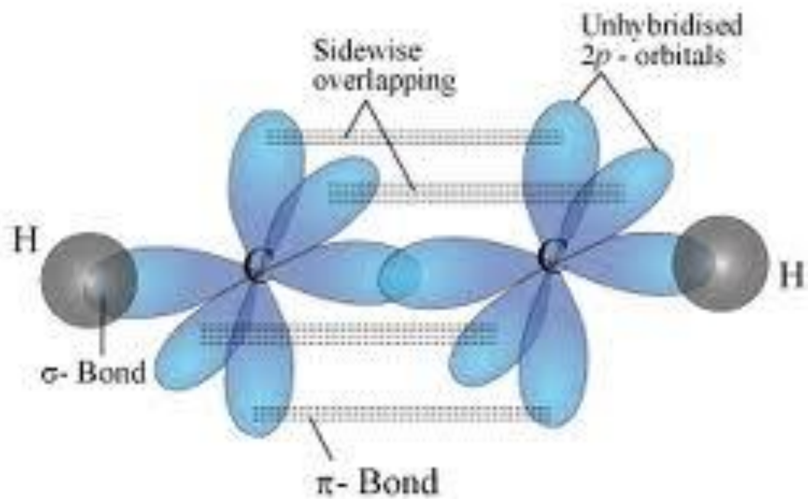


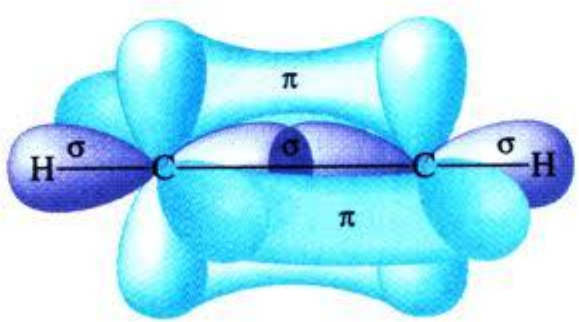
Figure 14 In an ethyne molecule, an *s* and a *p* orbital hybridize to form two *sp* hybrid orbitals (blue); two *p* orbitals remain (gold). The two *p* orbitals are 90° from each other.

Triple Bonds



$$H-C\equiv C-H$$

Sigma bonds form between:
•the sp orbital of one carbon with the sp orbital of the other carbon
•The sp orbital of each carbon and the s orbital of each hydrogen



Pi bonds form between:
•The p orbitals of the two carbon atoms

Summary

single bond	1 sigma bond
double bond	1 sigma bond 1 pi bond
triple bond	1 sigma bond 2 pi bonds

Practice

- Predict the hybridization and describe the three dimensional structure of propene

HOMEWORK

Required Reading:

p. 230-238

(remember to supplement your notes!)

Questions:

p. 238 #1-11