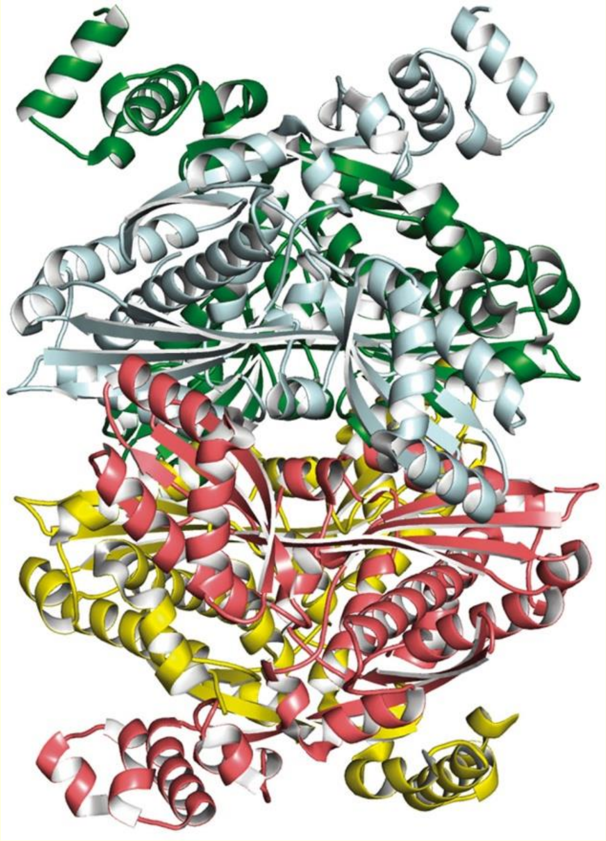
Structure and Bonding; Acids and Bases

스마트헬스케어학부 의공학전공

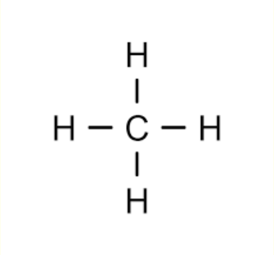
임해균 교수

1. Structure and Bonding; Acids and Bases

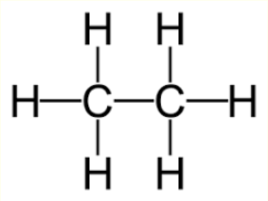


Orbitals and the Structure

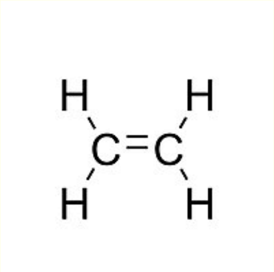
Methane
메테인



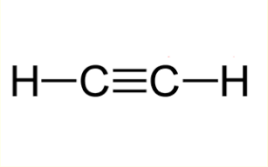
Ethane
에테인



Ethylene
(Ethene)
에틸렌



Acetylene
아세틸렌



1.6 *sp*^{3} Orbitals and the Structure of Methane

- Carbon has 4 valence electrons ($2s^2\ 2p^2$)
- In CH_4, all C–H bonds are identical (tetrahedral)
- ***sp*^{3} hybrid orbitals**: *s* orbital and three *p* orbitals combine to form four equivalent, unsymmetrical, tetrahedral orbitals (sppp = sp^3), Pauling (1931)

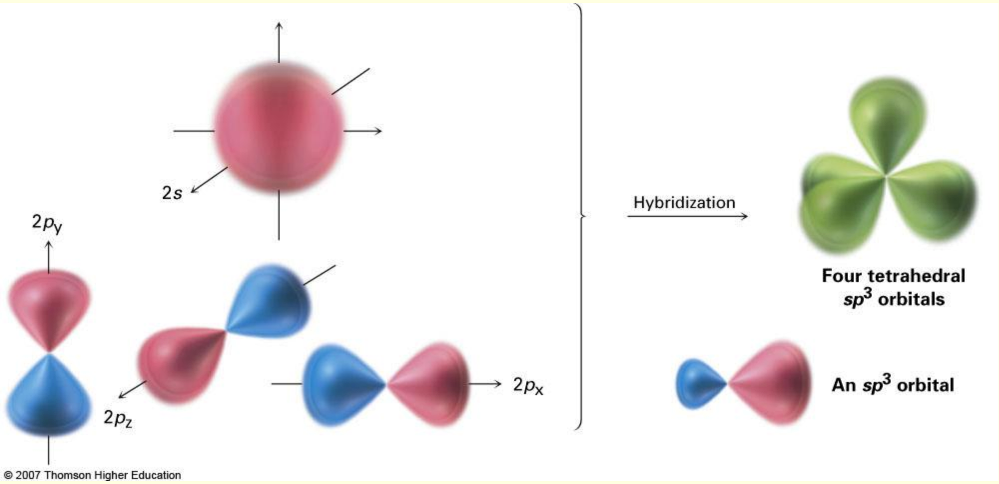
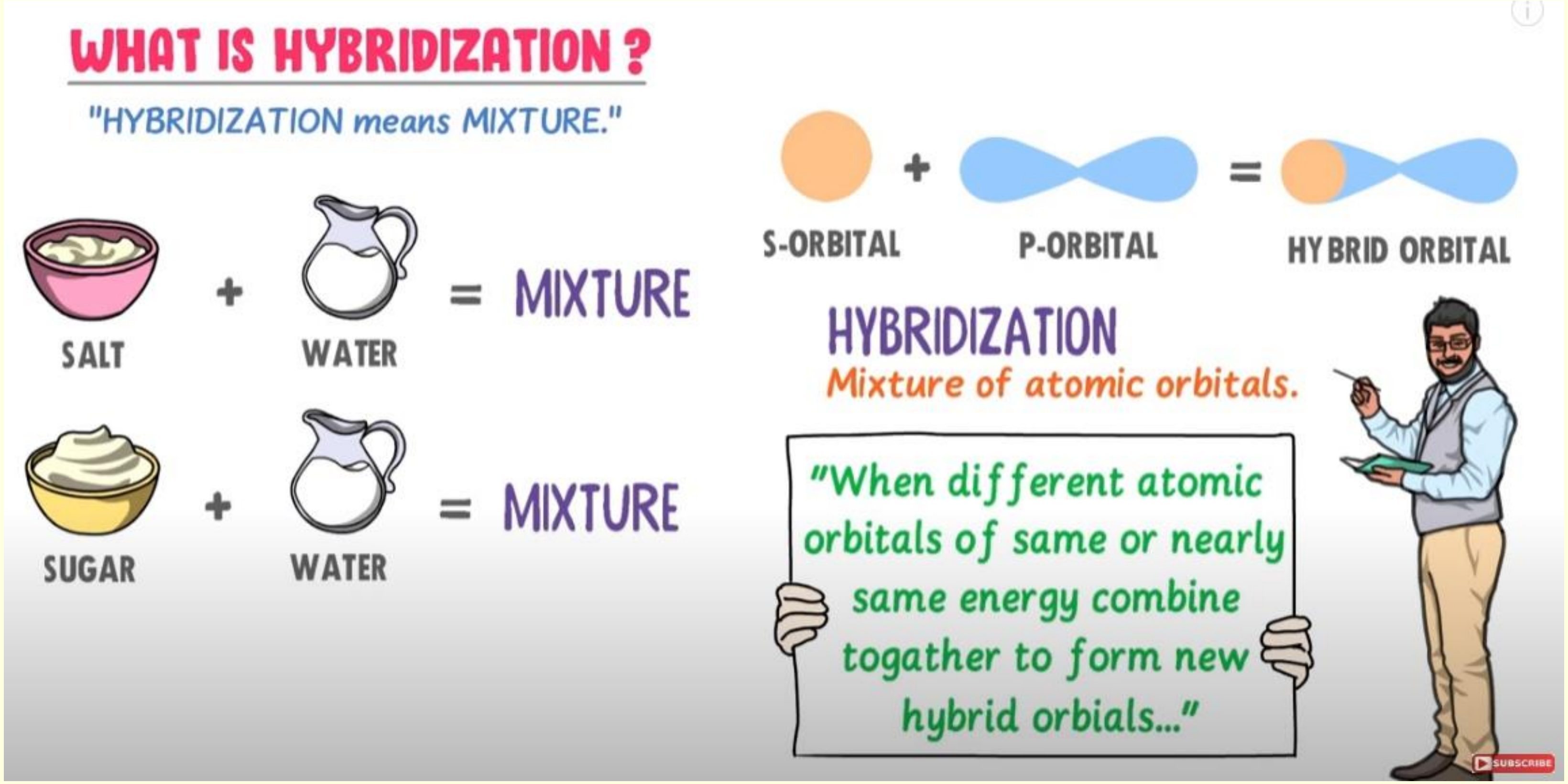


Figure 1.7 Four *sp*3 hybrid orbitals (green), oriented to the corners of a regular tetrahedron, are formed by combination of an atomic *s* orbital (red) and three atomic *p* orbitals (red/blue).

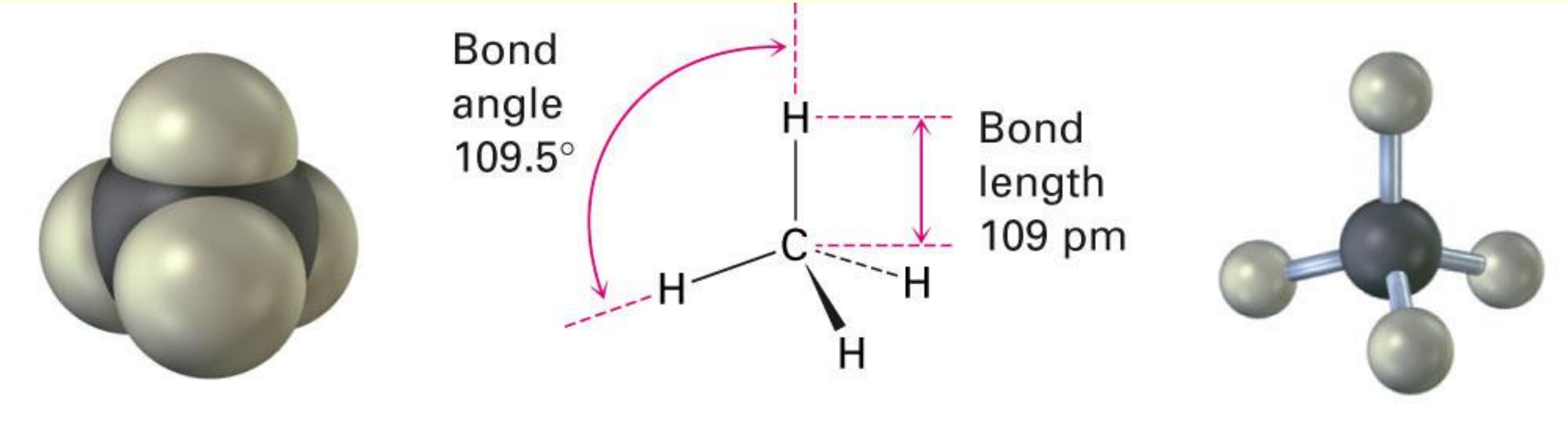
The *sp*3 hybrids have two lobes and are unsymmetrical about the nucleus, giving them a **directionality** and allowing them to **form strong bonds** when **they overlap an orbital from another atom.**

1.6 *sp*^{3} Orbitals and the Structure of Methane



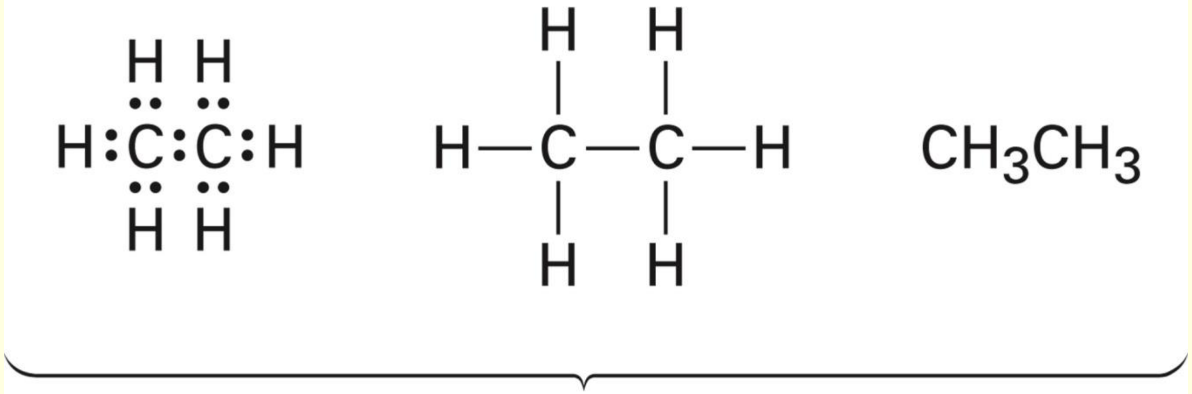
The Structure of Methane

- *sp*^{3} orbitals on **C overlap with 1*s* orbitals on 4 H atoms to form four identical C-H bonds**
- Each C–H bond has a strength of 439kJ/mol and length of 109 pm
- **Bond angle**: each H–C–H is 109.5°, the *tetrahedral angle*.



1.7 *sp*^{3} Orbitals and the Structure of Ethane

- Two C's bond to each other by σ overlap of an *sp*^{3} orbital from each
- Three *sp*^{3} orbitals on each C overlap with H 1*s* orbitals to form six C–H bonds
- C–H bond strength in ethane is 421 kJ/mol
- C–C bond is 154 pm long and strength is 376 kJ/mol
- All bond angles of ethane are tetrahedral



Some representations of ethane

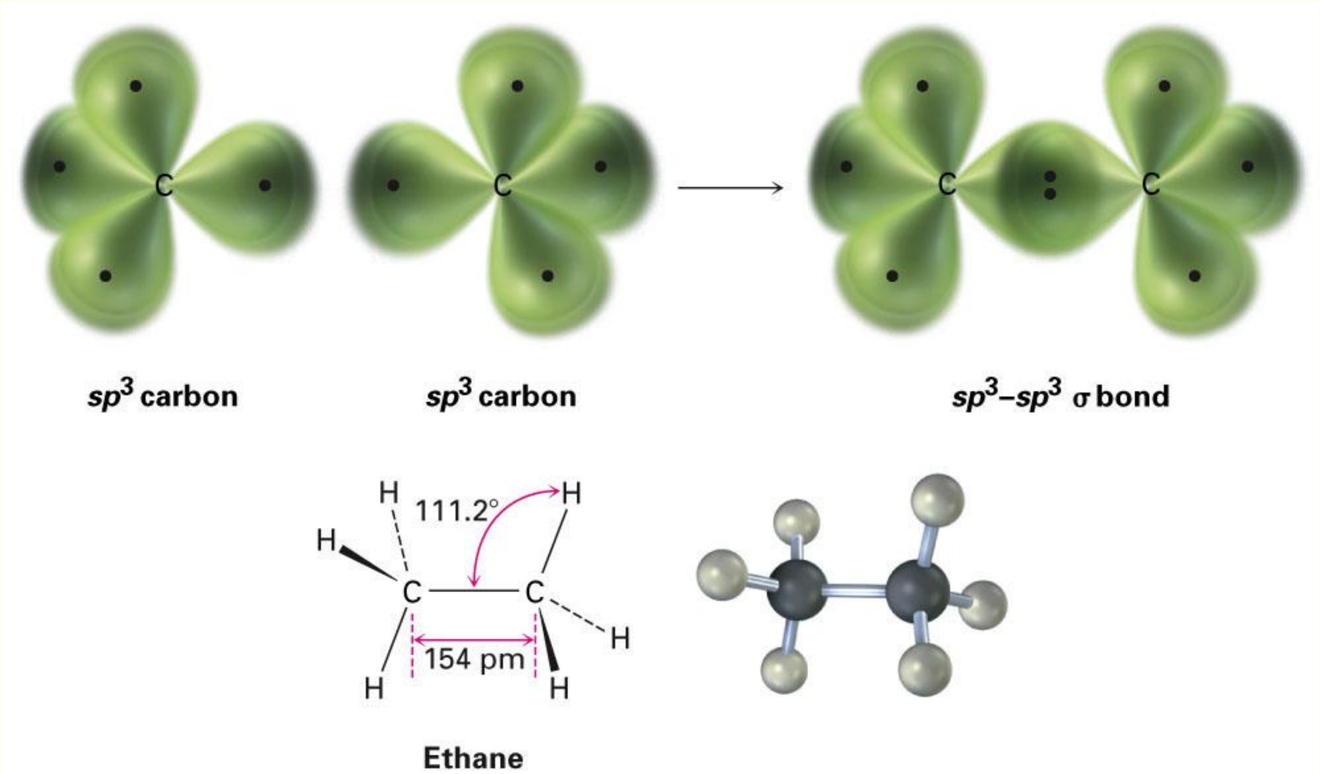
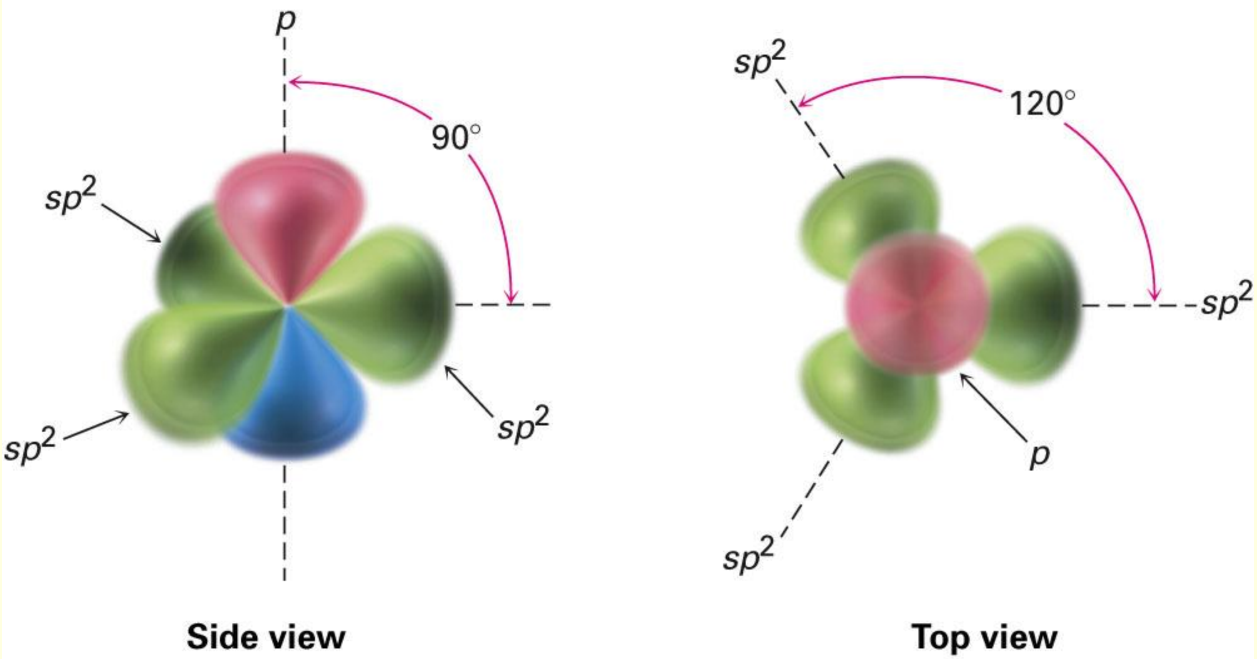


Figure 1.9 The structure of ethane.

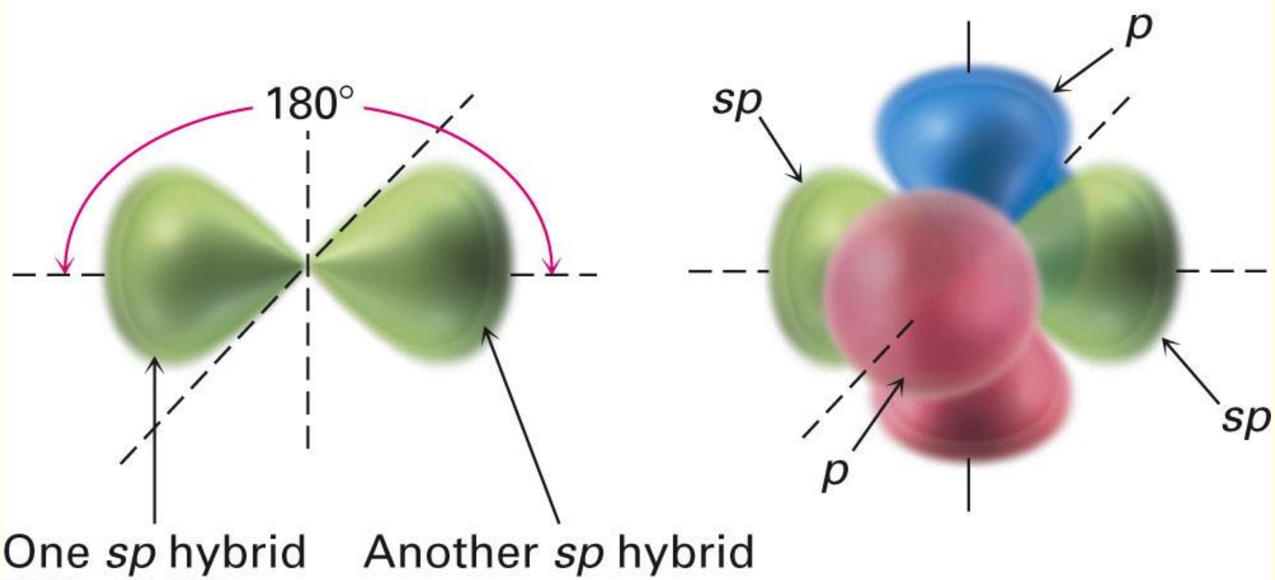
The carbon–carbon bond is formed by overlap of two carbon *sp*3 hybrid orbitals.
The C C bond is 154 pm long and has a strength of 377 kJ/mol (90 kcal/mol). All the bond angles of ethane are near, although not exactly at, the tetrahedral value of 109.5°.

1.8 Other Kinds of Hybrid Orbitals: *sp*^{2} and *sp*

- ***sp*^{2} hybrid orbitals:** 2*s* orbital combines with *two* 2*p* orbitals, giving 3 orbitals (spp = sp^2). This results in a double bond.
- *sp*^{2} orbitals are in a plane with120° angles
- Remaining *p* orbital is perpendicular to the plane

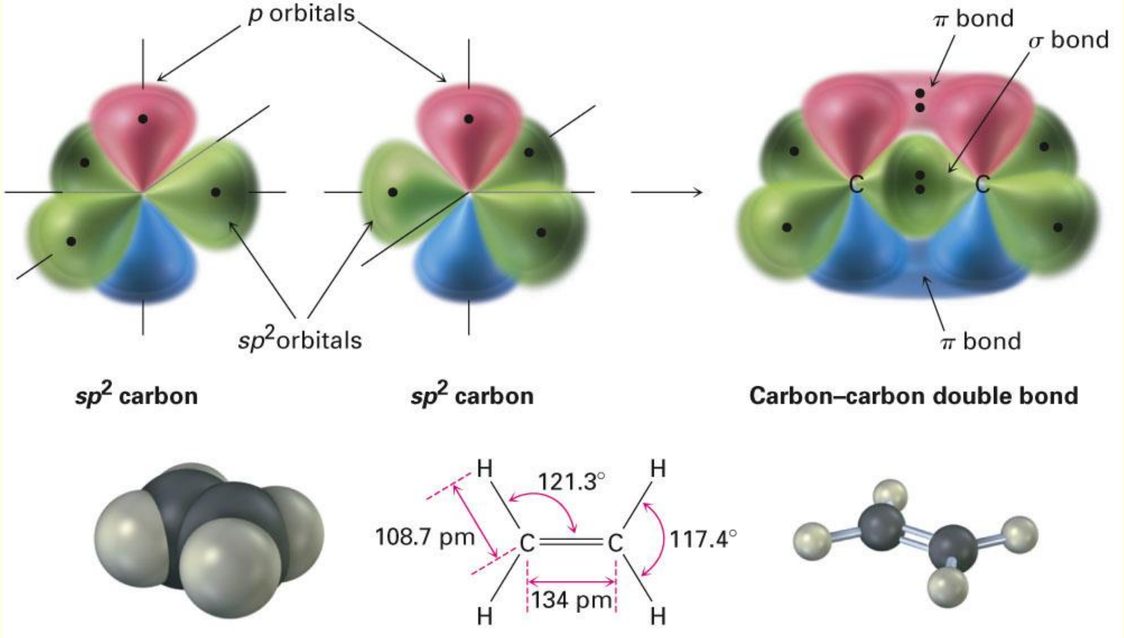


- ***sp* hybrid orbitals orbitals**
- C-C a *triple* bond sharing six electrons
- Carbon 2*s* orbital hybridizes with a single *p* orbital giving two *sp* hybrids
  - two *p* orbitals remain unchanged
- *sp* orbitals are linear, 180° apart on *x*-axis
- Two *p* orbitals are perpendicular on the *y*-axis and the *z*-axis



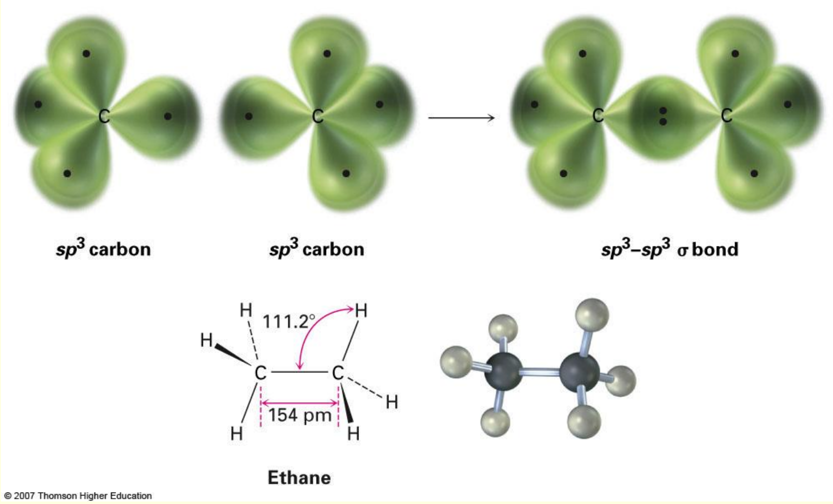
Bonds From sp^2 Hybrid Orbitals

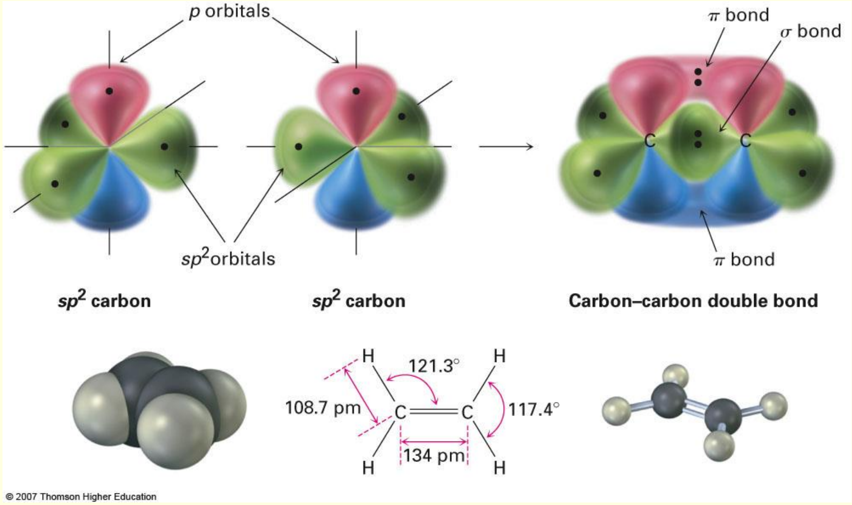
- Two *sp^2*-hybridized orbitals overlap to form a **sigma (σ) bond**
- *p* orbitals overlap *side-to-side* to formation a **pi (π) bond**
- *sp^2–sp^2* σ bond and 2*p*–2*p* π bond result in sharing four electrons and formation of C-C double bond
- Electrons in the σ bond are centered between nuclei
- Electrons in the π bond occupy regions are on either side of a line between nuclei



Structure of Ethylene

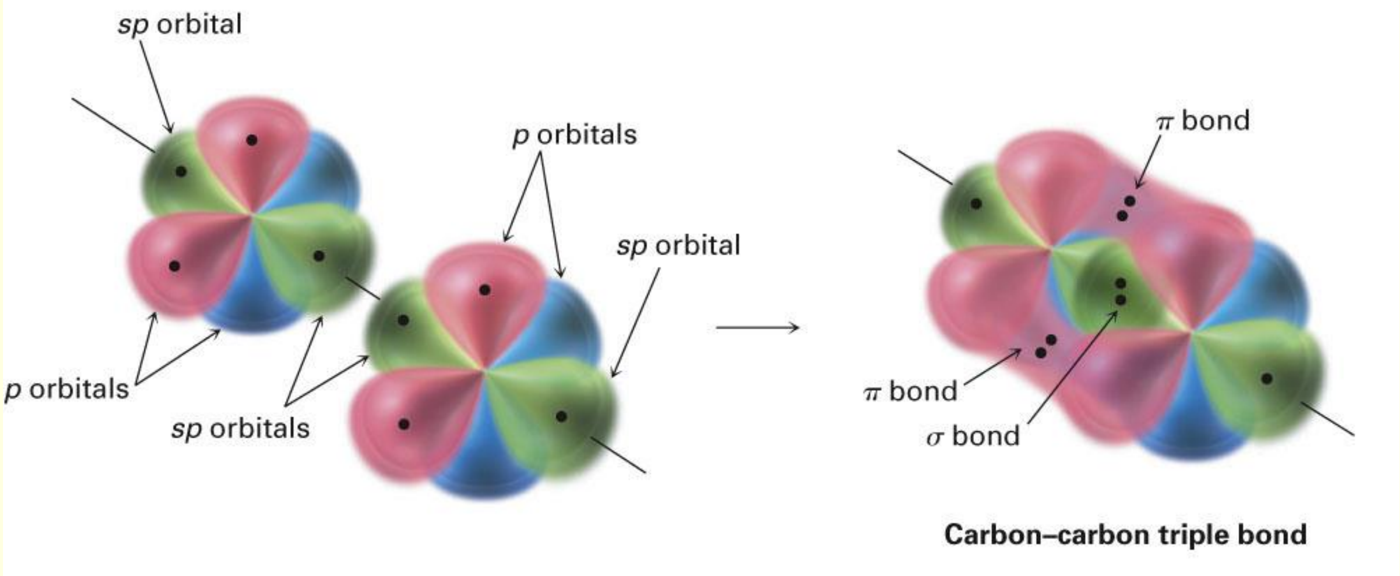
- H atoms form σ bonds with four sp^2 orbitals
- H–C–H and H–C–C bond angles of about 120°
- C–C double bond in ethylene shorter and stronger than single bond in ethane
- Ethylene C=C bond length 134 pm (C–C 154 pm)

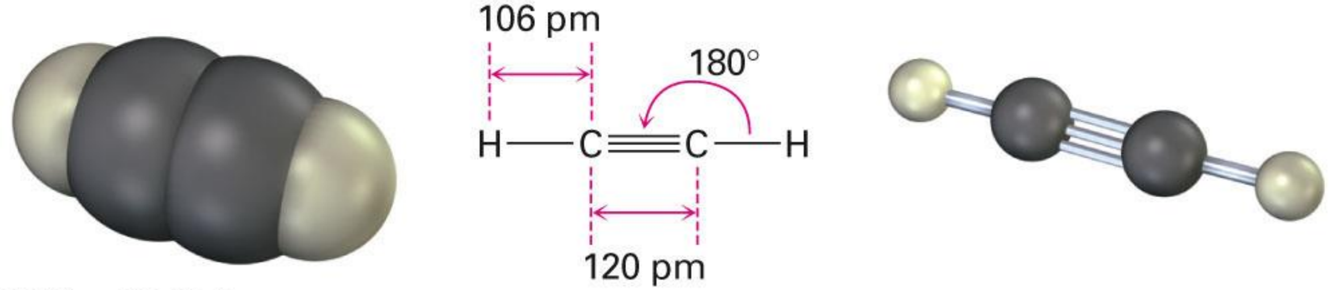


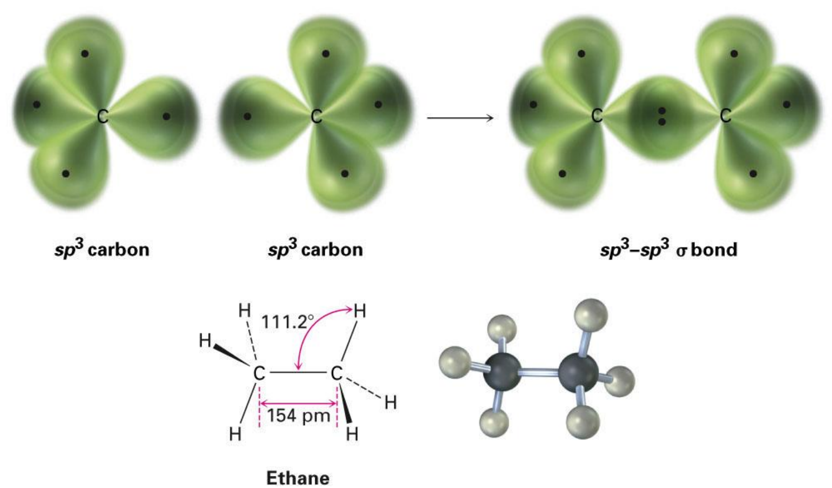


Structure of Acetylene

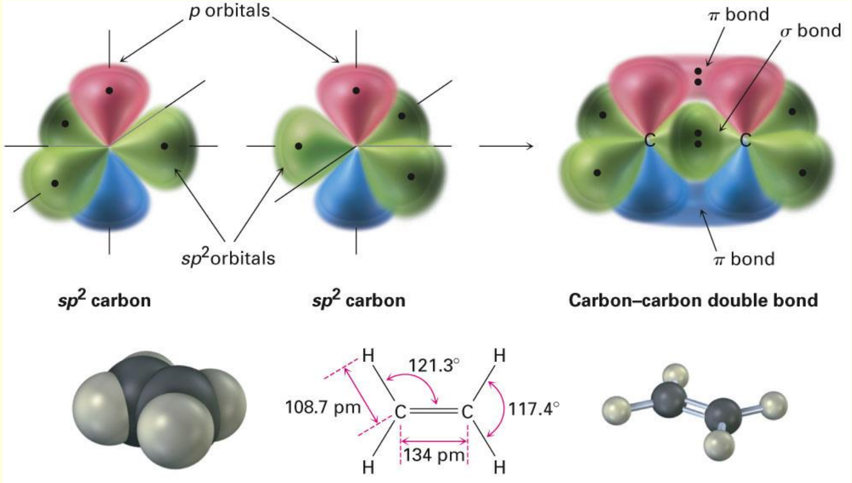
- Two *sp* hybrid orbitals from each C form *sp*–*sp* σ bond
- p_z orbitals from each C form a p_z–p_z π bond by sideways overlap and p_y orbitals overlap similarly



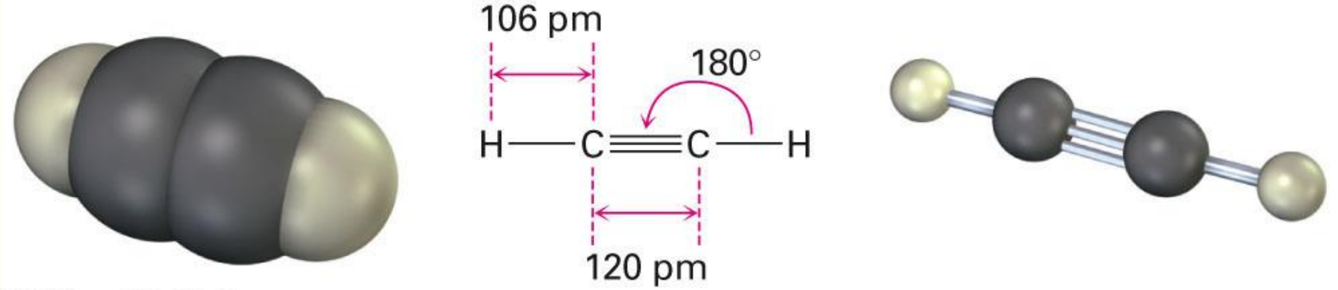




sp^3 carbon
sp^3 carbon
sp^3–sp^3 σ bond
111.2°
154 pm
Ethane



p orbitals
sp^2orbitals
π bond
σ bond
π bond
sp^2 carbon
sp^2 carbon
Carbon–carbon double bond
121.3°
108.7 pm
117.4°
134 pm



106 pm
180°
H—C≡C—H
120 pm

Worked Example 1.4

Drawing Electron-Dot and Line-Bond Structures

Formaldehyde, CH_2O, contains a carbon–*oxygen* double bond. Draw electron-dot and line-bond structures of formaldehyde, and indicate the hybridization of the carbon atom.

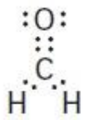
Worked Example 1.4

Drawing Electron-Dot and Line-Bond Structures

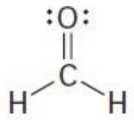
Formaldehyde, CH_2O, contains a carbon–*oxygen* double bond. Draw electron-dot and line-bond structures of formaldehyde, and indicate the hybridization of the carbon atom.

Strategy We know that hydrogen forms one covalent bond, carbon forms four, and oxygen forms two. Trial and error, combined with intuition, must be used to fit the atoms together.

Solution There is only one way that two hydrogens, one carbon, and one oxygen can combine:



Electron-dot structure



Line-bond structure

Like the carbon atoms in ethylene, the carbon atom in formaldehyde is sp^2-hybridized.