1.15
Bonding in Methane and Orbital Hybridization
Structure of Methane

tetrahedral
bond angles = 109.5°
bond distances = 110 pm
but structure seems inconsistent with electron configuration of carbon
Electron configuration of carbon

- Only two unpaired electrons should form $\sigma$ bonds to only two hydrogen atoms.
- Bonds should be at right angles to one another.

2p: Marked with two arrows pointing upwards.

2s: Marked with an arrow pointing downwards and one pointing upwards.
Promote an electron from the 2s to the 2p orbital
$sp^3$ Orbital Hybridization
Mix together (hybridize) the 2s orbital and the three 2p orbitals
Orbital Hybridization

$sp^3$ Orbital Hybridization

2 $sp^3$ orbitals

4 equivalent half-filled orbitals are consistent with four bonds and tetrahedral geometry

2 $p$ orbitals

2 $s$ orbital
Shapes of orbitals

$p$

$s$
Nodal properties of orbitals

$p$

$s$
Shape of sp$^3$ hybrid orbitals

$p$

take the s orbital and place it on top of the $p$ orbital

$s$
Shape of $sp^3$ hybrid orbitals

reinforcement of electron wave in regions where sign is the same

destructive interference in regions of opposite sign
Shape of $sp^3$ hybrid orbitals

orbital shown is $sp$ hybrid

analogous procedure using three $s$ orbitals and one $p$ orbital gives $sp^3$ hybrid

shape of $sp^3$ hybrid is similar
Hybrid orbital is not symmetrical

Higher probability of finding an electron on one side of the nucleus than the other

Leads to stronger bonds
The C—H σ Bond in Methane

In-phase overlap of a half-filled 1s orbital of hydrogen with a half-filled $sp^3$ hybrid orbital of carbon:

\[
\text{H} \quad \text{s} \quad \text{C} \quad \text{sp}^3
\]

gives a σ bond.

\[
\text{H—C} \quad \sigma
\]
Justification for Orbital Hybridization

consistent with structure of methane
allows for formation of 4 bonds rather than 2
bonds involving $sp^3$ hybrid orbitals are stronger than those involving $s-s$ overlap or $p-p$ overlap
1.16

$sp^3$ Hybridization

and Bonding in Ethane
Structure of Ethane

tetrahedral geometry at each carbon

C—H bond distance = 110 pm
C—C bond distance = 153 pm
The C—C $\sigma$ Bond in Ethane

In-phase overlap of half-filled $sp^3$ hybrid orbital of one carbon with half-filled $sp^3$ hybrid orbital of another.

Overlap is along internuclear axis to give a $\sigma$ bond.
The C—C $\sigma$ Bond in Ethane

In-phase overlap of half-filled $sp^3$ hybrid orbital of one carbon with half-filled $sp^3$ hybrid orbital of another. Overlap is along internuclear axis to give a $\sigma$ bond.
1.17

\( \text{sp}^2 \) Hybridization
and Bonding in Ethylene
Structure of Ethylene

$\text{C}_2\text{H}_4$

$\text{H}_2\text{C}=\text{CH}_2$

planar

bond angles: close to 120°

bond distances: $\text{C—H} = 110$ pm  
$\text{C}=\text{C} = 134$ pm
Promote an electron from the 2s to the 2p orbital
$sp^2$ Orbital Hybridization

$2p$  

$2s$  

$2p$  

$2s$
Mix together (hybridize) the 2s orbital and two of the three 2p orbitals
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**Orbital Hybridization**

2 $sp^2$ hybrid orbitals plus 1 $p$ orbital left unhybridized

3 equivalent half-filled $sp^2$ hybrid orbitals plus

$2p$
$sp^2$ Orbital Hybridization

2 of the 3 $sp^2$ orbitals are involved in $\sigma$ bonds to hydrogens; the other is involved in a $\sigma$ bond to carbon.
$sp^2$ Orbital Hybridization
\( \pi \text{ Bonding in Ethylene} \)

- The unhybridized \( p \) orbital of carbon is involved in \( \pi \) bonding to the other carbon.

\[ 2 \text{ } sp^2 \]

\[ p \]
each carbon has an unhybridized 2 \( p \) orbital

axis of orbital is perpendicular to the plane of the \( \sigma \) bonds
side-by-side overlap of half-filled $p$ orbitals gives a $\pi$ bond

double bond in ethylene has a $\sigma$ component and a $\pi$ component
1.18

$sp$ Hybridization

and Bonding in Acetylene
Structure of Acetylene

\[
C_2H_2
\]

HC≡CH

linear

bond angles: 180°

bond distances: C—H = 106 pm
              CC = 120 pm
Promote an electron from the 2s to the 2p orbital
sp Orbital Hybridization

$2p \uparrow \uparrow \downarrow \downarrow \quad 2p \uparrow \uparrow \uparrow \uparrow$

$2s \uparrow \downarrow \quad 2s \uparrow$
sp Orbital Hybridization

Mix together (hybridize) the 2s orbital and one of the three 2p orbitals
2 equivalent half-filled sp hybrid orbitals plus 2 p orbitals left unhybridized
Orbital Hybridization

2 sp

1 of the 2 sp orbitals is involved in a $\sigma$ bond to hydrogen; the other is involved in a $\sigma$ bond to carbon.
sp Orbital Hybridization

2 ρ

2 sp
**π Bonding in Acetylene**

The unhybridized $p$ orbitals of carbon are involved in separate $\pi$ bonds to the other carbon.
π Bonding in Acetylene

one π bond involves one of the p orbitals on each carbon
there is a second π bond perpendicular to this one
\( \pi \) Bonding in Acetylene

2 \( p \) bonds

2 \( sp \) bonds
π Bonding in Acetylene

2p

2sp
1.19
Which Theory of Chemical Bonding is Best?
Three Models

Lewis
most familiar—easiest to apply

Valence-Bond (Orbital Hybridization)
provides more insight than Lewis model
ability to connect structure and reactivity
to hybridization develops with practice

Molecular Orbital
potentially the most powerful method
but is the most abstract
requires the most experience to use effectively