Bonding in CH$_4$

How do we account for 4 C—H sigma bonds 109° apart?
We need to use 4 atomic orbitals — s, px, py, and pz — to form 4 new hybrid orbitals pointing in the correct direction.

s is spherical and the p orbitals are 90° apart — the hybridization changes the hybrid orbitals’ orientation.

Bonding in a Tetrahedron — Formation of Hybrid Atomic Orbitals

The C atom’s 4 orbitals hybridize to form four equivalent sp$^3$ hybrid molecular orbitals.

See CD-ROM screen 10.4
Orbital Hybridization

<table>
<thead>
<tr>
<th>#LP + ( \sigma )</th>
<th>SHAPE</th>
<th>ATOMIC ORB. USED</th>
<th>HYBRID ORBITALS</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>linear</td>
<td>s + p</td>
<td>sp</td>
</tr>
<tr>
<td>3</td>
<td>trigonal planar</td>
<td>s + 2 p</td>
<td>sp(^2)</td>
</tr>
<tr>
<td>4</td>
<td>tetrahedral</td>
<td>s + 3 p</td>
<td>sp(^3)</td>
</tr>
<tr>
<td>5</td>
<td>trigonal bipyramid</td>
<td>s + 3 p + d</td>
<td>sp(^3)d</td>
</tr>
<tr>
<td>6</td>
<td>octahedral</td>
<td>s + 3 p + 2 d</td>
<td>sp(^3)d(^2)</td>
</tr>
</tbody>
</table>

Multiple Bonds

Consider ethylene, C\(_2\)H\(_4\)

Trigonal planar around each C
There are 5 sigma bonds in C\textsubscript{2}H\textsubscript{4}, one of which is between Cs.

That means there is 1 pi bond in C\textsubscript{2}H\textsubscript{4}.

\[ \pi \text{ bond} \]

**\[ \pi \text{ Bonding in C}_2\text{H}_4 \]**

The unused p orbital on each C atom contains an electron and this p orbital overlaps the p orbital on the neighboring atom to form the \( \pi \) bond. (See Fig. 10.13)

2s
\[ \begin{array}{c}
\uparrow \\
n_{\text{orb.}}
\end{array} \]

2p
\[ \begin{array}{c}
\uparrow \uparrow \uparrow \uparrow \uparrow \\
3 \text{ sp}^2 \text{ hybrid orbitals for } \sigma \text{ bonds}
\end{array} \]

p orb.
\[ \begin{array}{c}
\uparrow \\
\text{for } \pi \text{ bond}
\end{array} \]
π Bonding in C₂H₄

The p orbital overlap that forms the π bond restricts rotation around the C=C bonds.

This is true of all double and triple bonds.

π Bonding in C₂H₂

Two p orbitals on each C overlap to form two π bonds, again restricting rotation around the C≡C bonds.
π Bonding in C$_2$H$_2$

\[
\begin{align*}
H & \quad \text{C} & \quad \text{C} & \quad \text{H} \\
\text{Side view} & \quad \text{End view} & \quad \text{Top view} \\
& \quad \text{π and σ bonds in a triple bond}
\end{align*}
\]

Consequences of Multiple Bonding

Restricted rotation around C=C bond.
π Bonding in C\textsubscript{6}H\textsubscript{6}

The sp\textsuperscript{3} hybridized C atoms have 1 p\textsubscript{z} orbital each. These overlap for each of 3 pairs of C atoms.

Two resonance forms lead to a delocalized π electron cloud
Benzene

σ bonds

π bonds

Complete bonding in benzene, $C_6H_6$

The energetics behind chemical reactions is also called thermodynamics, where “thermo” comes from the root for heat and “dynamics” comes from the root for change, thus thermodynamics means changes in the amount of heat (or energy) in a reaction.
Energy & Chemistry

- Burning peanuts supply sufficient energy to boil a cup of water.
- Burning sugar (sugar reacts with KClO₃, a strong oxidizing agent)

See screen 6.17 of the CD-ROM

Energy & Chemistry

\[ 2 \text{H}_2(g) + \text{O}_2(g) \rightarrow 2 \text{H}_2\text{O}(g) \quad \text{heat and light} \]

This reaction can be controlled to provide ELECTRIC ENERGY in a fuel cell, as is used on the space shuttle.

The chemical energy of combustion can be used to drive electrons in an electrical circuit.
ENERGY provides the capacity to do work or transfer heat.

HEAT is the form of energy that flows between 2 samples because of their difference in temperature.

Other forms of energy —
- light
- electrical
- mechanical

Potential energy — untapped energy available for future use. For a mass subject to gravity, this is energy the motionless mass has by virtue of its position.

See screen 6.2 of the CD-ROM
Kinetic and Potential Energy

**Kinetic energy** —
energy of motion.

• Translation
• Rotation
• Vibration

See screen 6.2 of the CD-ROM

Apr. 7, 2006

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Thermodynamics

• Thermodynamics is the science of heat (energy) transfer.

See screen 6.9 of the CD-ROM

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Heat energy is associated with molecular motion. The greater the motion, the hotter the substance.
Kinetic energy is associated with motion of a mass $m$ moving with a velocity $v$:

$$KE = \frac{1}{2} mv^2$$

The larger the mass $m$, the greater the kinetic energy. The higher the velocity $v$, the greater the kinetic energy.

As molecules bounce off each other, they transfer energy from more energetic molecules to less energetic molecules.

This slows the faster molecules and speeds the slower ones, leading to an equalization, or equilibrium.

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**UNITS OF ENERGY**

- 1 calorie = heat required to raise the temperature of 1 g of H$_2$O by 1.0 °C.
- 1000 cal = 1 kilocalorie = 1 kcal
- 1 kcal = 1 calorie (a food “calorie”)

The SI unit of energy is the JOULE

1 cal = 4.184 joules

A 2 kg mass moving at 1 m/sec has kinetic energy:

$$KE = \frac{1}{2} \times (2 \text{ kg}) \times (1 \text{ m/sec})^2 = 1 \text{ kg} \cdot \text{m}^2/\text{sec}^2 = 1 \text{ joule}$$