Lecture 32
Chapter 10  Sections 2-3

- Molecular orbitals
- Hybrid orbitals
- Multiple bonds
Announcements

• CAPA #17 due MONDAY!
• Seminar Friday 3:00 (physics)
• Seminar Friday 4:00 (chem/bio)

• CAPA #18 will be due after Thanksgiving (Tues or Wed)
• Exam #3 will be Friday 1 Dec. (Chapts 9-11, CAPAs 15-18)
• CAPA #19 will be due after the exam
Molecular Orbitals

- Bonding orbitals are constructed by combining atomic orbitals from adjacent atoms.
- Two atomic orbitals may be combined two ways: adding or subtracting.
- So, two 1s atomic orbitals on two Hs yield two molecular orbitals (MOs) in H₂.
- The whole H₂ molecule has two electrons, which we use to fill the MOs just as we filled atomic orbitals before.

![Diagram of bonding and anti-bonding orbitals](image)
Diatomic Molecules: HF and F₂

Strong 1s–2p overlap

Strong 2p–2p overlap
Orbitals and Shape

- OK, so we showed s and p orbitals making bonds
- But, we know something like methane is tetrahedral
- How do we get a tetrahedral shape from p orbitals?

- Well, we don’t.
- We need to come up with a slightly different picture that is mathematically equivalent to what we already have
- This is called **hybridization** and was first described by Linus Pauling
s and p hybridization

Diagram showing the process of hybridization involving 2s and 2p orbitals.
- CH₄ has tetrahedral structure…carbon is bonded to 4 hydrogen atoms.
- The s and all the p orbitals are needed for directional bonding, therefore, the s and the pₓ, pᵧ, and pₗ hybridize.
- The new orbitals are called sp³.
- Any inner atom with a steric number of 4 has tetrahedral electron group geometry and can be described using sp³ hybrid orbitals.
What a second…

• This seems like we are just making this up because we know methane is supposed to be tetrahedral.

• Not really, there is lots of fancy math underneath hybridization that we aren’t showing you (yet).

• It turns out that it is mathematically equivalent to have one s and three p orbitals or four sp³ orbitals.

• So, the two descriptions are mathematically identical – sometimes one is easier to visualize than another.
General Features of Hybridization

1. The number of valence orbitals generated by the hybridization process equals the number of valence atomic orbitals participating in hybridization.
   - Orbitals are modified – not created or destroyed
2. The steric number of an inner atom uniquely determines the number and type of hybrid orbitals.
3. Hybrid orbitals form localized bonds by overlap with atomic orbitals or with other hybrid orbitals.
4. There is no need to hybridize orbitals on outer atoms, because atoms do not have limiting geometries. Hydrogen always forms localized bonds with its 1s orbital. The bonds formed by all other outer atoms can be described using valence p orbitals.
Methanol

C–O Bond

Inner atom orbitals

Methanol
**sp² hybrid orbitals**

- Mixes an s orbital with two p orbitals \((s+p+p)\)
- Utilized by central atoms with steric number of 3 (trigonal planar electron group geometry)
sp hybrid orbitals

- Mixes an s orbital with a p orbital (s+p)
- Utilized by central atoms with steric number of 2 (linear electron group geometry)

![Diagram showing the mixing of s and p orbitals to form sp hybrid orbitals.](image)
What is the hybridization of the atom labeled 5 in acetic acid?

25%  A. s
25%  B. p
25%  C. sp2
25%  D. sp3
What is the hybridization of the atom labeled 1 in acetic acid?

25% A. s
25% B. p
25% C. sp2
25% D. sp3
What is the hybridization of the atom labeled 7 in acetic acid?

A. s  
B. p  
C. sp²  
D. sp³
sp\(^3\)d hybrid orbitals

- Mixes an s orbital with three p orbitals and a d orbital (s+p+p+p+d)
- Utilized by central atoms with steric number of 5 (trigonal bipyramidal electron group geometry)
\( \text{sp}^{3}\text{d}^2 \)

- Mixes an s orbital with three p orbitals and two d orbitals \((s+p+p+p+d+d)\)
- Utilized by central atoms with steric number of 6 (octahedral electron group geometry)
# Table 10 – 1: Summary of Valence Orbital Hybridization

<table>
<thead>
<tr>
<th>Steric Number</th>
<th>Electron Group Geometry</th>
<th>Hybridization</th>
<th>Number of Hybrid Orbitals</th>
<th>Number of Unused p Orbitals</th>
<th>Picture</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Linear</td>
<td>$sp$</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Trigonal planar</td>
<td>$sp^2$</td>
<td>3</td>
<td>1</td>
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<tr>
<td>4</td>
<td>Tetrahedral</td>
<td>$sp^3$</td>
<td>4</td>
<td>0</td>
<td><img src="image2.png" alt="Picture" /></td>
</tr>
<tr>
<td>5</td>
<td>Trigonal bipyramidal</td>
<td>$sp^3d$</td>
<td>5</td>
<td>0</td>
<td><img src="image3.png" alt="Picture" /></td>
</tr>
<tr>
<td>6</td>
<td>Octahedral</td>
<td>$sp^3d^2$</td>
<td>6</td>
<td>0</td>
<td><img src="image4.png" alt="Picture" /></td>
</tr>
</tbody>
</table>
Sigma ($\sigma$) bonds

- All bonds we have seen so far have been $\sigma$ bonds
- **Electron density lies on the bond axis, between the atoms**
How do we form double bonds?

- We have used up the space between the nuclei for the sigma bond.
- We must form multiple bonds from orbitals that look different
- Look at ethene for example

Lewis structure

Ball-and-stick Model

C–H bonds: $1s$–$sp^2$ overlap

C–C bond: $sp^2$–$sp^2$ overlap
Pi (\(\pi\)) bonds – from p orbitals

- P orbitals not involved in hybridization can form \(\pi\) bonds
- \(\pi\) bonds have electron density above and below the bond axis, not between them

![Oblique view](image1)

![Top view](image2)

![End view](image3)

![Side view](image4)
Ethene

Lewis structure

Ball-and-stick Model

Top view

Side view

End view
What about triple bonds?

- Ethyne has sp-hybridization
- This leaves two p orbitals on each C free for π-bonding
Molecular Orbitals – revisited

\[ \text{H}_2 \]

\[ \text{He}_2 \]

\[ \text{He}_2^+ \]
Is the bond in $\text{H}_2^-$ stronger or weaker than the bond in $\text{H}_2$?

50%  1. Weaker
50%  2. Stronger
Today

- Physics seminar 3:00
- Chem/Bio seminar 4:00 (VDW 102)

Monday

- Finish CAPA #17

Remember: You are done with the homework when you understand it!