Lecture 28
Chapter 9  Sections 3-4

- Resonance
- VSEPR – molecular shape
Announcements

• CAPA #16 due Monday
• Seminars today 3:00 and 4:00
• Seminar next Tuesday at 11:00
Example for you: phosphoric acid $\text{H}_3\text{PO}_4$

BUILDING LEWIS STRUCTURES

Step 1  Count the valence electrons.
Step 2  Assemble the bonding framework, placing two electrons per bond.
Step 3  Place three nonbonding pairs of on electrons each outer atom, except H.
Step 4  Assign the remaining valence electrons to inner atoms.
Step 5  Optimize electron configurations of the inner atoms.
Step 6  Identify equivalent or near-equivalent Lewis structures.
What is the formal charge on P in $\text{H}_3\text{PO}_4$?

<table>
<thead>
<tr>
<th>Percentage</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>20%</td>
<td>1. -2</td>
</tr>
<tr>
<td>20%</td>
<td>2. -1</td>
</tr>
<tr>
<td>20%</td>
<td>3. 0</td>
</tr>
<tr>
<td>20%</td>
<td>4. 1</td>
</tr>
<tr>
<td>20%</td>
<td>5. 2</td>
</tr>
</tbody>
</table>
Resonance

- When multiple, equivalent Lewis structures may be drawn
- Resonance indicates stability
Example for you: $\text{CO}_3^{2-}$

**BUILDING LEWIS STRUCTURES**

**Step 1** Count the valence electrons.

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**Step 4** Assign the remaining valence electrons to inner atoms.

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**Step 6** Identify equivalent or near-equivalent Lewis structures.
How many resonance structures can you draw for $\text{CO}_3^{2-}$?

- 20% 1. zero
- 20% 2. one
- 20% 3. two
- 20% 4. three
- 20% 5. four
Molecular Shapes
Electron Pair Repulsion

• Molecules have three dimensional shape.
  – The 3-D shape defines the properties of the molecules.
• How do we predict the shape?
• **VSEPR Theory** – valence shell electron-pair repulsion theory
  – Electron pairs in the outer shell of an atom try to get as far away from each other as possible
  – Why? Because like charges repel…they want to be far away from each other.
• The result? 2 electron pairs ➔ line
  3 electron pairs ➔ trigonal planar (triangle)
  4 electron pairs ➔ tetrahedron (pyramid)
Electron pairs get away from each other

Two C–H bonds optimally separated in space.

Three C–H bonds optimally separated in space.

Four C–H bonds optimally separated in space.

2 electron ‘groups’

3 electron groups

4 electron groups
• In the plane of the paper, it looks like the bond angles are 90°.
• But, we know that the molecule exists in three dimensions.
• The bonds are really optimized around the central carbon.
• The shape is called tetrahedral and has bond angles of 109.5°.
Carbon and the Tetrahedron

- Carbon often forms molecules based on tetrahedral shape.
  - This is because C often bonds to four neighbors.

- Hydrocarbons – molecules that contain only carbon and hydrogen
- Alkanes – hydrocarbons in which each carbon atom forms four single bonds to other atoms.

(a) Ethane

(a) Propane
Back to the VSEPR Model

- First some definitions:
  - **Electron group** – a set of electrons that occupies a particular region around an atom. (usually a lone pair or a bonding pair)
  - **Ligand** – an atom or a group of atoms bonded to an inner atom
  - **Steric number** – the sum of the number of ligands plus the number of lone pairs; in other words, the total number of groups of electrons associated with that atom.
• All molecules above have the same steric number.

• **Electron group geometry** – is the 3-D arrangement of the valence shell electron groups, corresponds to the steric number
Molecular Shape

- The molecular shape describes how the ligands (not the electron groups) are arranged in space.
- This group of molecules all have different shapes.
- Electron groups all feel each other, but we can “see” only atoms

Steric number = 4
Electron group geometry = Tetrahedral

Tetrahedral

CH$_4$
Ligands = 4
Lone pairs = 0

Trigonal pyramidal

NH$_3$
Ligands = 3
Lone pairs = 1

Bent

H$_2$O
Ligands = 2
Lone pairs = 2
DETERMINING MOLECULAR SHAPES

**Step 1** Determine the Lewis structure.

**Step 2** Use the Lewis structure to find steric numbers for inner atoms.

**Step 3** Determine electron group geometries from steric numbers.

**Step 4** Use the ligand count to derive molecular shapes from electron group geometries.
Example – $\text{H}_3\text{O}^+$

- What is the steric number? Four
- Electron group shape? Tetrahedral
- How many ligands? Three
- Molecular shape? Trigonal pyramid
Other Molecular Shapes – p. 366-371

- Steric Number 2: **Linear Electron Group Geometry**

\[ \text{O} = \text{C} = \text{O} \]

- Coordination number = 2
- Steric number = 2

- Linear molecular shape
- Bond angle = 180°
More Molecular Shapes – p. 366-371

- Steric Number 3: Trigonal Planar Electron Group Geometry

Each C atom has
Steric number = 3

Each C atom has
Trigonal planar geometry
More Molecular Shapes – p. 366-371

• Steric Number 5: Trigonal Bipyramidal Electron Group Geometry

Steric number = 5
Electron group geometry = Trigonal bipyramidal

<table>
<thead>
<tr>
<th></th>
<th>PCl$_5$</th>
<th>SF$_4$</th>
<th>ClF$_3$</th>
<th>I$_3^-$</th>
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</thead>
<tbody>
<tr>
<td>Ligands</td>
<td>5</td>
<td>4</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Lone pairs</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>
More Molecular Shapes – p. 366-371

• Steric Number 6: Octahedral Electron Group Geometry

Steric number = 6
Electron group geometry = Octahedral

Octahedral

\[ \text{SF}_6 \]
Ligands = 6
Lone pairs = 0

Square pyramidal

\[ \text{ClF}_5 \]
Ligands = 5
Lone pairs = 1

Square planar

\[ \text{XeF}_4 \]
Ligands = 4
Lone pairs = 2
Today

- Two seminars
  - 3:00 SC1019
  - 4:00 SC1000

Monday

- CAPA #16 due
- Seminar Tuesday 11:00

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