Lecture 28
Chapter 9  Sections 3-4

• Resonance
• VSEPR – molecular shape
Announcements

• CAPA due Thursday
• Seminar tomorrow 11:00
• Seminar Friday 4:00
• Seminar next Tuesday at 11:00
Example for you: phosphoric acid  $\text{H}_3\text{PO}_4$

<table>
<thead>
<tr>
<th>Step 1</th>
<th>Count the valence electrons.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 2</td>
<td>Assemble the bonding framework, placing two electrons per bond.</td>
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<td>Place three nonbonding pairs of on electrons each outer atom, except H.</td>
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<td>Step 5</td>
<td>Optimize electron configurations of the inner atoms.</td>
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<td>Step 6</td>
<td>Identify equivalent or near-equivalent Lewis structures.</td>
</tr>
</tbody>
</table>
What is the formal charge on P in H$_3$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.
- **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.
How many resonance structures can you draw for 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.
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.
Electron Group Geometry

Steric number = 4
Electron group geometry = Tetrahedral

- 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

| CH₄ | LH = 4 | Lone pairs = 0 |

Trigonal pyramidal

| NH₃ | LH = 3 | Lone pairs = 1 |

Bent

| H₂O | LH = 2 | Lone pairs = 2 |
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

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

Coordination number = 2
Steric number = 2

Linear molecular shape
Bond angle = 180°
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

- **Trigonal bipyramidal**
  - $\text{PCl}_5$
  - Ligands = 5
  - Lone pairs = 0

- **Seesaw**
  - $\text{SF}_4$
  - Ligands = 4
  - Lone pairs = 1

- **T-shaped**
  - $\text{ClF}_3$
  - Ligands = 3
  - Lone pairs = 2

- **Linear**
  - $\text{I}_3^-$
  - Ligands = 2
  - Lone pairs = 1
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
• Finish CAPA

Thursday
• Seminar 11:00
• CAPA

Friday
• Seminar 4:00

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