Recitation Activity 8 (Chapter 9)

1. VESPR model

For each compound below draw the Lewis Structure and fill in the blanks

<table>
<thead>
<tr>
<th></th>
<th>#Bonded Pairs</th>
<th>#Lone Pairs</th>
<th>E- domain Shape</th>
<th>Molecular Shape</th>
<th>Polar/nonpolar</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}_2\text{S} )</td>
<td>4</td>
<td>2</td>
<td>tetrahedral</td>
<td>bent</td>
<td>polar</td>
</tr>
<tr>
<td>( \text{SeO}_3^{2-} )</td>
<td>3</td>
<td>1</td>
<td>tetrahedral</td>
<td>trigonal</td>
<td>polar</td>
</tr>
<tr>
<td>( \text{IF}_4^+ )</td>
<td>4</td>
<td>1</td>
<td>trigonal</td>
<td>seesaw</td>
<td>polar</td>
</tr>
<tr>
<td>( \text{SF}_6 )</td>
<td>6</td>
<td>6</td>
<td>octahedral</td>
<td>octahedral</td>
<td>nonpolar</td>
</tr>
</tbody>
</table>

2. Valence Bond model and Hybridization

For each compound below:

a. Draw the Lewis Structure (including resonance forms if appropriate)

b. Determine the number and label the sigma and pi bonds.

c. For each atom with more than one neighbor:
   • Determine the hybridization
   • Give the approximate bond angles
   • Determine the hybridization at each central atom
There are three resonance structures: each of which contains three single bonds and one pi bond. Because the central atom (carbon) forms three sigma bonds the hybridization at that carbon is sp², and the 3rd p-orbital on carbon is used to make the delocalized pi bond. The geometry of the carbonate ion is trigonal planar, with O-C-O bond angles equal to exactly 120°.

**Acrylonitrile:**

\[ \text{sp hybridization, 180° bond angles, linear geometry} \]

\[ \text{sp}^2 \text{ hybridization, 120° bond angles, trigonal planar geometry} \]

\[ \text{sp}^2 \text{ hybridization, 120° bond angles, trigonal planar geometry} \]

3. Molecular Orbitals and Bond Order

Use the MO diagram in Figure 9.38 (p348) to describe the bonding in O₂⁺, O₂, and O₂⁻. Which of the three should be stable? What is the bond order of each? Which contain unpaired electrons?

\[
\text{Bond order} = \frac{1}{2} (\# \text{bonding electrons} - \# \text{nonbonding electrons}) \\
O_2^+ = \frac{1}{2} \left( 8-3 \right) = 2.5 \text{ (1 unpaired electron)} \\
O_2 = \frac{1}{2} \left( 8-4 \right) = 2 \text{ (2 unpaired electrons)} \\
O_2^- = \frac{1}{2} \left( 8-5 \right) = 1.5 \text{ (1 unpaired electron)}
\]

Since the bond order is greater than zero in all three cases, each is stable with respect to no bond at all.
4. There are three possible structures (called "isomers") for dichloroethylene, \( \text{C}_2\text{H}_2\text{Cl}_2 \), two of which are polar and one which is not.

a) Draw the three Lewis structures (use the name to help you), predict an overall shape for each and explain why one is nonpolar and the others are polar.

b) Two of the three structures can be interconverted by a process called cis-trans\(^*\) isomerization, in which rotation about the central carbon-carbon bond takes places upon irradiation with UV light. If light with a wavelength of approximately 200 nm is required for isomerization, how much energy (in kJ/mol) is this?

c) Finally, sketch the orbitals involved in the carbon-carbon bond, and explain why so much energy is necessary for the bond rotation to occur.

\(^*\)"Cis" refers to the chlorines being on the same side of the molecule and 'trans' means they are on opposite sides.

\[
\begin{array}{ccc}
\text{H} & \text{H} & \text{H} & \text{Cl} & \text{H} & \text{Cl} \\
\text{\hspace{1cm}} / & / & / & / & / & / \\
\text{C} & = & \text{C} & \text{C} & = & \text{C} \\
\text{\hspace{1cm}} / & \text{\hspace{1cm}} / & \text{\hspace{1cm}} / & \text{\hspace{1cm}} / & \text{\hspace{1cm}} / & \text{\hspace{1cm}} / \\
\text{Cl} & \text{Cl} & \text{Cl} & \text{H} & \text{H} & \text{Cl} \\
\text{Polar} & \text{Nonpolar} & \text{Polar} \\
\end{array}
\]

\[
E = \frac{hc}{\lambda} \times N = \left(\frac{6.626 \times 10^{-34} \text{Js} \times 3.00 \times 10^8 \text{ms}^{-1}}{200 \times 10^{-9} \text{m}}\right) \times (6.022 \times 10^{23} \text{photons/mole}) = 599 \text{kJ/mol}.
\]

It takes this fairly large packet of energy for bond rotation because the \( \pi \) bond must be broken before rotation can occur.
5. Imagine your sister is majoring in chemistry at OSU and is completing her last lab experiment before graduating. She was given an unknown and asked to determine its molecular formula and crystal structure using X-ray fluorescence and X-ray diffraction. The notes in her lab book read as follows:

**X-ray fluorescence spectroscopy** reveals that the stoichiometry is $\text{MX}_4$, but the resolution of the instrument is not sufficient to distinguish between neighboring elements. Your sister only knows that $\text{M}$ is either: Te, I or Xe, and that $\text{X}$ is either: O or F.

**X-ray diffraction analysis** reveals that crystal structure contains planar $\text{MX}_4$ molecules, with the $\text{M}$ in the center of the molecule, $\text{M-X}$ bond distances of 2.02 Å and the $\text{X-M-X}$ bond angles that are all either 90° or 180°.

As a lowly freshman or sophomore can you help your sister graduate by identifying her unknown compound, thereby freeing up your parents tuition money next quarter to be lavished upon you.

*Only XeF$_4$ could be square planar.*

**Additional thought—provoking questions**

What is the more common name for ‘square bipyramidal’ geometry?

*Square bipyramidal.*

The word “pyramid” implies a three dimensional structure while “trigonal” or “square” implies 2D, i.e. the base plane. The octahedron is two pyramids each of which is sitting on a square base (just like the Egyptian pyramids). The trigonal bipyramidal is two pyramids each of which is sitting on a triangular base.