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Week 1

Friday, October 2

▷ Determining formal charge:

◦ Formula: $FC = V - N - \frac{B}{2}$

◦ V = valence electrons of element

◦ N = lone pair electrons; B = bonded electrons

1. What is the formal charge on P in the following structure? Each F and O has three lone pair of electrons.

◦ $P = 5 - 0 - 8(0.5)$; P = **+1**

2. What is the formal charge on O in the structure above?

◦ $O = 6 - 6 - 2(0.5)$; O = **-1**

3. What is the formal charge on P in the following structure? Each F still has three lone pairs of electrons, and O had the two pairs indicated.

◦ $P = 5 - 0 - 10(0.5)$; P = **0**

4. Of the two structures shown for POF_3 , which is the most stable, and will, therefore, be the most abundant form?

◦ **Structure II**

◦ O has formal charge of **0** and is the **most electronegative** element with difference in charge between the resonance structures.

◦ F has greater electronegativity, but remains the same between both structures, so it's not relevant.

◦ Key difference: the double bond in structure II gives oxygen the **lower magnitude** formal charge between the two.

5. The fundamental concept upon which VSEPR, and hence molecular shapes, is based is that:

◦ Electrons pairs repel each other;

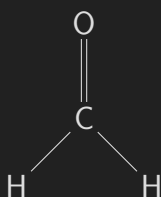
– negative charge repels other negative charges.

◦ Electron repulsion is minimized by maximum angular separation;

– in other words, angular separation maximizes distance between electrons.

◦ Bonding pair electrons and lone pair electrons both occupy regions around the central atom;

- if they didn't occupy the same space than they wouldn't interact and thus wouldn't affect shape.
 - The electron domain geometry and the molecular geometry is identical if there all of the electrons are bonding electrons;
 - the lone pairs are have a greater influence than bonded pairs, resulting in less space for bonded pairs.
 - **All of the above**
- ▷ General method of determining structure:
1. Count steric number—the total number of electron pairs in a molecule. Can be bonds or lone pairs.
 2. Determine predicted geometrical structure predicted (EDG) by VSEPR using steric number.
 - Octahedral:6, Bipyramid:5, Tetrahedral:4, Trigonal:3, Linear:2
 3. Determin impact (the MG) of lone pairs; more lone pairs results in less space between bonded pairs. Shape depends on EDG.
6. A resonance form of SOF_2 , completely consistent with the octet rule, is shown below. What is the electron domain geometry (EDG), and molecular geometry (MG) of this molecule?
- **Tetrahedral EDG and trigonal pyramidal MG**
7. Draw a Lewis dot structure of formaldehyde (CH_2O): what is the molecular shape of this molecule?



- Steric number = 3
 - Double bonds count as 1 for steric number.
 - No lone pairs on central atom, C, so it's shape planar.
 - **Trigonal planar**
8. The EDG for CH_3^- (a carbanion) is tetrahedral, and the MG is trigonal pyramidal. Why are the $\text{H}-\text{C}-\text{H}$ bond angles less than 109.5° as in a perfect tetrahedron?
- **The lone pair electrons take up more space than bonding pair electrons.**

Week 2

Monday, October 5

1. The concept of orbital shapes comes directly from the wave model of the atom. What is the shape of an s orbital?

- ▷ **Spherical**

- S orbital is the most simple orbital, with only two electrons.
- Alternative shapes come from *nodes*; i.e. when *destructive interferences* cancels out the wave function.
- Not circular, orbitals are three-dimensional.

2. What is the shape of a p orbital?

- ▷ **Dumbbell shaped**

- P orbital can hold 6 electrons (3 pairs).
- Each pair has one angular node, squeezing shape into dumbbell in each direction (x, y, z).

3. When atomic orbitals overlap to form a covalent bond, the resultant bonding orbital is:

- ▷ **Lower in energy than the atomic orbitals from which it was formed**

- Electrons in a covalent bond are in a more stable (lower energy) state due to multiple nuclei holding them in place.
- Only when nodes are present do the electrons create a destabilized molecular orbit, increasing the energy.

4. Why can't pure p orbitals be used in forming four equivalent bonds as in methane?

- ▷ the three 2p orbitals can only hold 6 electrons.

- True, we need to make four bonds for methane.

- ▷ the bonds would have to be 90° apart.

- If p had enough space then it would result in planar geometry with 90°, but the true arrangement is tetrahedral with angles of 109.5°

- ▷ electron-electron repulsion would not be minimized.

- Planar minimization would be 90°, but we have 3d space to work with, so it's not minimized.

- ▷ **all of the above**

5. When s and p orbitals combine to form hybrid orbitals, the resultant hybridized orbitals are:

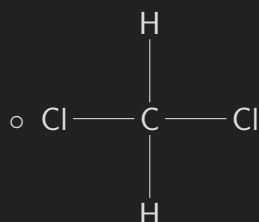
- ▷ lower in energy than the p orbitals
- ▷ higher in energy than the s orbitals
- ▷ **both of the above**
 - It takes energy to move the electron up from the s orbital and hybridize the p orbitals.
 - The new hybridized sp orbital also has more energy than the s orbital.

6. What is the difference between a sigma bond and a pi bond?

- ▷ **in a π bond, electron density lies above and below the axis that connects the two nuclei; in a σ bond, the electronegative density lies along the axis that connects the two nuclei**
 - σ bond has circular symmetry with respect to the bond axis (axis that connects the two nuclei). i.e. it's along the axis.

7. What is the hybridization of the C in CH₂Cl₂?

▷ **sp³**



- Look at central atom – C
- Determine groups (number of bonds, π bonds count as 1, and lone pairs attached) – 4
- for groups 1-4; sp^x; x = groups - 1 (**3**)
- This is also a trigonal planar, due to lone pairs on Cl I guess? (lone pairs not drawn)

8. What is the hybridization of each C in benzene (shown below)?

▷ **sp²**

- Each carbon has 2H and π bond between, so groups = 3.
- Groups - 1 = 2, so sp²
- Though, each π bond is delocalized, or free to spread across all the carbons. Still counts as 1 group.

Wednesday, October 7



Friday, October 9

