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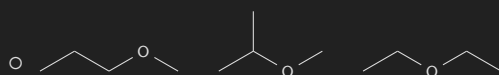
Week 3

Monday, October 12

1. How many isomers exist for a molecule with the molecular formula $C_4H_{10}O$?

   ▷ **7**
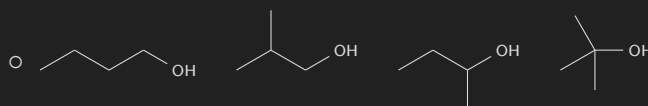
   - These are the alcohols, or *all the possbile combinations where the oxygen is on the end*? (? I'm sure when we get into nomenclature this will make more senses and lead to better explanation)

   - These are the ethers, or *all the possbile combinations where the oxygen is within the chain*? (? same disclaimer as above)

   ○ Seems like drawing is only way to get good at this. Eventually we will probably get some intuition or memorize certain compounds with continual practice, similar to practicing math problems.

2. How many degrees of unsaturation are there in $C_4H_{10}O$?

   ▷ **0**

   ○ Determining saturation using molecular formula: C_nH_{2n+2}
   n = carbon atoms.

   - **Halogens**: takes the place of a hydrogen atom; add one H for each halogen.

   - **Oxygen**: no affect on saturation; ignore.

   - **Nitrogen**: needs an extra hydrogen; subtract one H for each nitrogen.

   ○ Or use HDI formula: HDI = $\frac{1}{2}(2C + 2 + N - H - X)$ X: halogen atoms.

   - HDI: hydrogen deficiency index, which is the measure of degrees of freedom.

   - For $C_4H_{10}O$: $\frac{1}{2}(8 + 2 + 0 - 10 - 0) = \frac{1}{2}(0) = 0$

3. Based upon the previous question, which structure(s) can be eliminated as possible for $C_4H_{10}O$?

   ▷ **all of the above**

     ○ Zero degrees of freedom means no double/triple bonds or rings are possbile.

     ○ Degrees of freedom help represent possbile structures, indicating possible double bounds, triple bounds, rings, or various combinations of each.

4. How many degrees of unsaturation are there in C_5H_{13}?

   ▷ **0**

     ○ Again, general formula: HDI = $\frac{1}{2}(2C + 2 + N - H - X)$ X: halogen atoms.

     ○ For $C_5H_{13}N$: $\frac{1}{2}(2(5) + 2 + 1 - 13 - 0) = \frac{1}{2}(0) = 0$

5. Based upon the previous question, what is a possible structure for $C_5H_{13}N$?

   ▷

     ○ Same as question three, zero degrees of freedom means no double/triple bonds or rings are possbile.
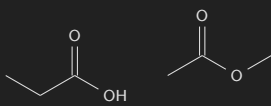
6. How many degrees of unsaturation exist for a molecule with the formula $C_3H_6O_2$?

   ▷ **1**

     ○ $\frac{1}{2}(2(3) + 2 + 0 - 6 - 0) = \frac{1}{2}(2) = 1$

7. What structures are possible for the $C_3H_6O_2$ molecule?
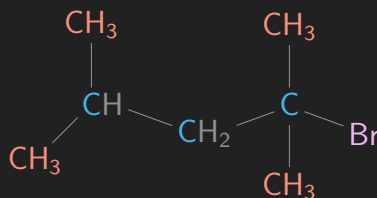
   ▷ **both the first and second structures are possible**

     ○ For reference:

     ○ Has one degree of freedom so it has to have at least a double/triple bound or ring structure.

       – Makes invalid due to lack of any double/triple/rings.
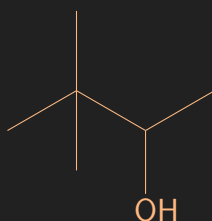
Week 2

Friday, October 9

1. What is the condensed formula for the following molecule?

   ▷ **$(CH_3)_2CHCH_2C(CH_3)_2Br$**

      ○ Breaking down answer: $(CH_3)_2CHCH_2C(CH_3)_2Br$

2. What is the structural formula for $(CH_3)_3CCH(OH)CH_3$?

   ▷ Each line with an end is a CH_3 (need 4)

   ▷ Three points touching is a CH. (need 1)

   ▷ (OH) is on the CH

3. For any two molecules to be constitutional isomers of each other, at the very least, they:

   ▷ **must have the same chemical formula**

      ○ isomers: same chemical formula.

      ○ constitution: ways it connects; connect must be different to be a constitutional isomer.

4. How many constitutional isomers can be formed with the molecular formula $C_4H_{10}O$?

   ▷ **7**

      ○ See Monday, October 12 quiz. Same question asked and a better explanation given there.

5. The SO2 molecule has two resonance forms, each of which is a constitutional isomer of the other. Which of the two structures shown below is the most stable? (The S→O bond is a dative bond in which both bonding electrons come from only one atom.)
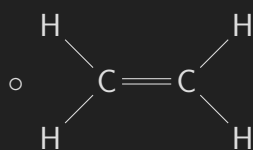
▷ **the structure on the right**

○ *Delocalized electrons being shared in multiple bonds are more stable than a the dative bond.*[?] (? Not sufficient enough information yet to be confident of this explanation, though I'd be willing to bet that its along the right lines)

Wednesday, October 7

1. What is the hybridization of the orbitals on C in ethylene?

   ▷ **sp^2**

   ○
   $$H\diagdown\quad\quad\diagup H$$
   $$C = C$$
   $$H\diagup\quad\quad\diagdown H$$

   ○ Each C has 3 groups (number of bonds, π bonds count as 1, or lone pairs)

   ○ For atoms with groups between 1 and 4; sp^x; x = groups - 1 = (2)

2. What is the hybridization of the orbitals on C in acetylene?

   ▷ **sp**

   ○ H — C $\equiv$ C — H

   ○ 2 groups, thus x = 1.

3. What type of bonds combine to make a C=C double bond?

   ▷ **one sigma and one pi bond.**

   ○ First bond is a σ bond.

   ○ Additional bonds are π bonds that go above and below the axis that connects the nuclei.

4. What is the H-C-H bond angle in ethylene?

   ▷ **120°**

   ○ sp^2 with no lone pairs, thus trigonal planar (according to VSEPR).

   ○ $\frac{360}{3}$ = 120; 3 angles maximized on a single plane.

5. Why is the geometry around the CH2 fragment in ethylene, trigonal planar?

   ▷ **there are three regions of electron density**

   ○ *regions electron density =$^?$ groups* (? I'm combining a past youtube video with his lecture...)

6. There is completely free rotation around a sigma bond such as a C−C single bond. Propose a reason for why there is no free rotation around a C=C.

   ▷ **the rotation would require the C−C pi bond to break**

   ○ σ bonds can rotate on the axis between the nuclei, but the π bonds are above and below and would break during rotation since *there are*

other orbitals that would block[?] their rotation. (? not completely sure on the mechanism that doesn't allow for rotation)

7. As the percent s character increases in a bond, what happens to the bond angle?

   ▷ **it increases**

      ○ The more *s* character, the shorter and stronger the bond, and the larger the bond angle.

8. As the percent p character in a bond increases, what happens to the bond angle?

   ▷ **it decreases**

      ○ the more p character, the less s character; inverse of s character.

9. Why is a pi bond weaker than a sigma bond?

   ▷ **all of the above**

10. Which statement(s) is(are) correct?

   ▷ the shorter the bond, the stronger the bond

   ▷ the more s character in the hybridization, the stronger the bond

   ▷ the more s character in the hybridization, the greater the bond angle

   ▷ sigma bonds are stronger than pi bonds

   ▷ the geometry around the C in the ethylene is trigonal planar

   ▷ a C=C bond is composed of one sigma and one pi bond

   ▷ the hybridization around C in the methyl anion, isoelectronic with CH_4, is sp^3

   ▷ when 2s and 2p orbitals mix to form hybrid orbitals, the hybrid orbitals are higher in energy than the 2s orbitals, but lower in energy than the 2p orbitals

   ▷ the shapres of the hybrid orbitals match the electron domain geometry shapes predicted by VSEPR

   ▷ the potential energy of a covalent bond is lower than that of the potential energies of the free atoms from which it was formed

   ▷ **ALL OR THE ABOVE**

      ○ This seems to be a review of important concepts.

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?

   ▷ **Dumbell shaped**

      ○ P orbital can hold 6 electrons (3 pairs).

      ○ Each pair has one angular node, squeezing shape into dumbell 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 hodling them in place.

      ○ Only when nodes are present do the electrons create a destabalized molecular orbit, incraseing 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 conects the two nuclei; in a σ bond, the electronegative density lies along the axis that connets the two nuclei**

      ○ σ bond has circular symmetry with respect to the bond axis (axis that connets the two nuclei). i.e. it's along the axis.

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

   ▷ **sp^3**

      ○
```
            H
            |
    Cl ─── C ─── Cl
            |
            H
```
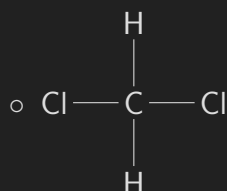
      ○ Look at central atom — C

      ○ Determin groups (number of bonds, π bonds count as 1, and lone pairs attached) — 4

      ○ for groups 1-4; sp^x; x = groups - 1 (3)

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

   ▷ **sp^2**

      ○ Each carbon has 2H and π bond between, so groups = 3.

      ○ Groups - 1 = 2, so sp^2

      ○ Though, each π bond is delocalized, or free to spread across all the carbons. Still counts as 1 group.

Week 1

Friday, October 2

▷ Determing formal charge:

- Formula: $FC = V - N - \dfrac{B}{2}$
- V = valance 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 tow 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 dommain 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 geomterical 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?
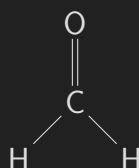
    - Steric number = 3

        - 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 $H-C-H$ bond angles less than **109.5°** as in a perfect tetrahedron?

- The lone pair electrons take up more space than bonding pair electrons.