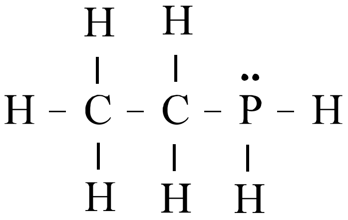
Dr. Zellmer
Time: 7 PM Sun.
30 min

Chemistry 1210
Autumn Semester 2022
Quiz X

All Sections
November 13, 2022

Name KEY Rec. TA/time

1. (3 pts) For $CH_3CH_2PH_2$ what are the molecular shapes around the C and P atoms, in the order given in the molecule, left to right?



$$\begin{array}{ccccccccc} & & \mathrm{H} & & \mathrm{H} & & & & \\ & & | & & | & & \cdot\cdot & & \\ \mathrm{H} & - & \mathrm{C} & - & \mathrm{C} & - & \mathrm{P} & - & \mathrm{H} \\ & & | & & | & & | & & \\ & & \mathrm{H} & & \mathrm{H} & & \mathrm{H} & & \end{array}$$

(polar)

Shape around:

C atoms: **tetrahedral -** 4 atoms attached to the C atoms and no lone pairs, bond angles around C are ~109.5° and it is polar around the C atoms.

P atom: **trigonal pyramidal -** 3 atoms and 1 lone pair of electrons on the P atom. Since the electron-pair arrangement around the P atom is tetrahedral but all 4 things on the P atom are not identical the molecule will have bond angles of ~109.5° and it will be polar around the P atom. Around the P atom it looks like PH_3 and NH_3 but with one of the H atoms replaced with the CH_3CH_2- group.

2. (3 pts) Which hybrid orbitals lead to a **<u>bent</u>** shape with bond angles of about 105°?

a) sp b) sp^2 c)* sp^3 d) sp^3d e) sp^2d

sp^3 hybrid orbitals give an electron-domain tetrahedral geometry with angles of 109.5°. When an atom has 4 things around it the atom generally is using **sp^3** hybrid orbitals for bonding. The **bent** shape arises when an atom is bonded to 2 other atoms and has 2 lpe^- on it (4 things total). An example is H_2O. The O atom is sp^3 hybridized and uses two of the hybrid orbitals to form the bonds to the H atoms and two sp^3 hybrid orbitals are used for the lpe^- on the O atom. The two lpe^- spread out and force the H atoms closer together. For a central atom from period 2, each lpe^- reduces the bond angle by about 2°.

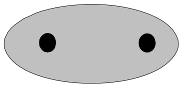
The hybrid orbital give the electron-domain geometries and bond angles below:

sp	linear, 180°
sp^2	trigonal planar, 120° (molecular shapes: trigonal planar, bent)
sp^3	tetrahedral, 109.5° (molecular shapes: tetrahedral, trigonal pyramidal, bent)

You don't have to invoke hybridizations of sp^3d and sp^3d^2 to get the trigonal pyramidal and octahedral geometries as pointed out in the textbook. Some books use these types of hybrid orbitals to explain these geometries but our book doesn't.

3. (3 pts) Describe what a sigma, σ, bond is and what a pi, π , bond is in terms of their electron density. Sketch what a pi bond between two atoms looks like (use two large dots to represent the nucleus of each atom).

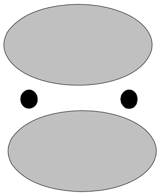
σ bond



Electron density concentrated along the internuclear axis, mostly between the two nuclei. Sigma bonds result from the following types of overlap,

- s - s (like between H atoms in H_2)
- s - p (end on)
- p - p (end on)
- s - hybrid (end on)
- p - hybrid (end on)
- hybrid - hybrid (end on)

π bond



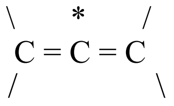
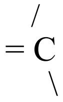
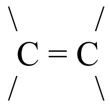
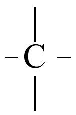
Two lobes with electron density lying above and below the internuclear axis. Pi (π) bonds result from the sideways overlap of two p orbitals, one on each atom, which are perpendicular to the internuclear axis.

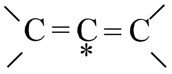
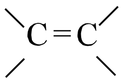
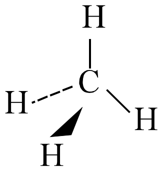
4. (3 pts) How many **sp** hybridized carbon atoms are contained in the following compound?

$$H - \overset{sp}{C} \equiv \overset{sp}{C} - \overset{sp^3}{CH_2} - \overset{sp}{C} \equiv \overset{sp}{C} - \overset{sp^3}{CH_2} - \overset{sp}{C} \equiv \overset{sp}{C} - \overset{sp^2}{CH} = \overset{sp^2}{CH} - \overset{sp^3}{CH_2} - \overset{sp^2}{CH} = \overset{sp^2}{CH} - \overset{sp^3}{CH_3}$$

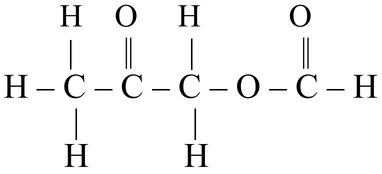
The carbon atoms in the triple bond form 2 ***sp*** hybrid orbitals each with two *p* orbitals remaining . The ***sp*** orbitals form a σ bond with hydrogen and/or with carbon atoms (total of 2 σ bonds). The other two bonds between the carbon atoms results from a side-by-side overlap of the two *p* orbitals of each carbon atom to form two pi (π) bonds. The molecule above has 4 sp^3, 4 sp^2 and 6 ***sp*** hybridized C atoms.

The molecule above has 3 triple bonds. Since each triple bond has two sp hybridized carbon atoms, there are a total of 6 sp hybridized carbon atoms. (Remember, each triple bond has 2 ***sp*** hybridized orbitals and two p orbitals). The double-bonded C atoms each have only 1 double bond to them so there are 4 sp^2 hybridized carbon atoms (Remember, each "normal" double bond has 2 sp^2 hybridized carbon atoms; see exception below). Normally carbon atoms with double bonds are sp^2 hybridized. However, there is an exception when a carbon atom has 2 double bonds to it (the 2nd carbon from the right). In this case the carbon atom is ***sp*** hybridized (see below).

– C ≡ C –	sp hybrid carbon atoms
	sp hybrid carbon atom (= $\overset{*}{C}$ = in middle,  is sp^2)
	sp^2 hybridized carbon (2 single bonds and double bond to carbon)
	sp^3 (4 single bonds)

–C≡C– or 	2 things attached to a central atom	sp hybridization linear, 180°
	3 things attached to a central atom	sp^2 hybridization trigonal planar, 120°
	4 things attached to a central atom	sp^3 hybridization tetrahedral, 109.5°

5. (7 pts) For the following molecule (draw in any lone-pair electrons not shown), what are the total number of σ and π bonds in the molecule? **Explain your answers.**



$$\mathrm{H-\overset{H}{\underset{H}{C}}-\overset{O}{\overset{\|}{C}}-\overset{H}{\underset{H}{C}}-O-\overset{O}{\overset{\|}{C}}-H}$$

Single bonds are σ bonds.

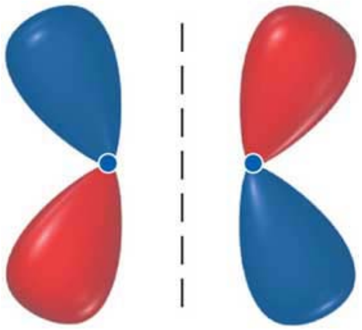
Also, σ bonds appear in double and triple bonds.

A double bond consists of 1 σ bond and 1 π bond.

A triple bond consists of 1 σ bond and 2 π bonds.

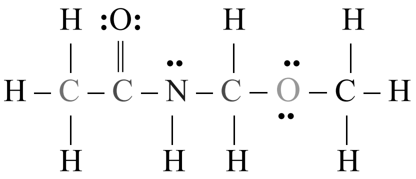
12 σ bonds & 2 π bonds

4. (2 pts) Consider the following figure. This is a (sigma or pi), (bonding or antibonding) molecular orbital.

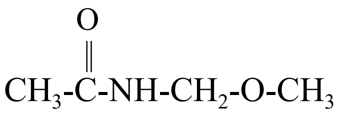


This is a pi antibonding MO. It results from the destructive sideways overlap (add out of phase) of atomic p orbitals. When this happens you get an antibonding MO with a node between the two nuclei (there is also a node along the internuclear axis because p atomic orbitals have a planar node between the 2 lobes, the figure above doesn't really show that well but it's the dots in the middle). See Section 9.8, Figure 9.36 and the Closer Look box (Phases in atomic and molecular orbitals) in this section for more information.

7. (6 pts) For the following molecule (draw in any lone-pair electrons not shown) answer the questions below. **Explain your answers.**



$$\begin{array}{ccccccccccccccc} & & H & & :O: & & & & H & & & & H & & \\ & & | & & \| & & \cdot\cdot & & | & & \cdot\cdot & & | & & \\ H & - & C & - & C & - & N & - & C & - & O & - & C & - & H \\ & & | & & & & | & & | & & \cdot\cdot & & | & & \\ & & H & & & & H & & H & & & & H & & \end{array}$$



$CH_3\text{-}\overset{\overset{O}{\|}}{C}\text{-}NH\text{-}CH_2\text{-}O\text{-}CH_3$ (Condensed formula)

a) What are the hybridizations of all the central atoms left to right?

CH_3 carbon atom on the far left: **sp^3**, the C is bonded to 4 other atoms, tetrahedral and has to be sp^3 hybridized. (4 single bonds, which are σ bonds).

C = O carbon atom: **sp^2**, the C is bonded to 3 other atoms so it's trigonal planar so has to be sp^2 hybridized. (3 σ bonds and 1 π bond to the C).

C – **N** – C nitrogen atom: **sp^3**, the N has 4 things around it (2 C atoms, 1 lone-pair and 1 H atom), it has to have a tetrahedral electron domain and thus has to be sp^3 hybridized.

N – **C** – O carbon atom: **sp^3**, the C is bonded to 4 other atoms, tetrahedral and has to be sp^3 hybridized. (4 single bonds, which are σ bonds)

C – **O** – C oxygen atom: **sp^3**, the O has 4 things around it (2 C atoms and 2 lone-pairs), it has to have a tetrahedral electron domain and thus has to be sp^3 hybridized.

CH_3 carbon atom on the far right: **sp^3**, the C is bonded to 4 other atoms, tetrahedral and has to be sp^3 hybridized. (4 single bonds, which are σ bonds).

b) What are the bond angles around all the central atoms from left to right?

H – **C** – C (1st C atom on the left): The C atom is bonded to 4 atoms so its ED geometry and molecular geom are both tetrahedral with a bond angle of ~ **109.5°**.

C – **C** – N (2nd C atom from left): This C atom is bonded to 3 atoms (no lpe^-) and is has a trigonal planar geometry so the bonds around it are ~ **120°**.

C – **N** – C (the N atom): The N atom is bonded to 3 atoms and has 1 lpe^- so its ED geometry is tetrahedral with a molecular geometry of trigonal pyramidal (like NH_3) and a bond angle of ~ **109.5°**.

N – **C** – O (C atom between N & O atoms): The C atom is bonded to 4 atoms so its ED geometry and molecular geom are both tetrahedral with a bond angle of ~ **109.5°**.

C – **O** – C (O atom between the two C atoms on the right): The **O** atom is bonded to 2atoms and has 2 lpe^- so its ED geometry is tetrahedral with a molecular geometry of trigonal pyramidal (like NH_3) and a bond angle of ~ **109.5°**.

O – **C** – H (C atom on the far right): The C atom is bonded to 4 atoms so its ED geometry and molecular geom are both tetrahedral with a bond angle of ~ **109.5°**.

8. (8 pts) Using the appropriate **MO diagram**, for each of the following, give the **bond order** and whether it is paramagnetic **or** diamagnetic (and how you know this).

I'm using the MO electron configurations like I did in class rather than drawing out the MO diagrams every time.

a) C_2^+ # e^- = 2*6 - 1 = 11 (this is the total number of valence electrons)

$(\sigma_{1s})^2(\sigma_{1s}*)^2(\sigma_{2s})^2(\sigma_{2s}*)^2(\pi_{2p})^3(\sigma_{2p})^0(\pi_{2p}*)^0(\sigma_{2p}*)^0$ (don't need empty orbitals)

$KK(\sigma_{2s})^2(\sigma_{2s}*)^2(\pi_{2p})^3$ shorthand

(replace both σ_{1s} with K and leave off empty orbitals - not asked for)

B.O. = ½ (# bonding electrons − # anti-bonding electrons)

= ½ (7 − 4) = **1.5** (smaller B.O. than C_2)

Can use just the valence electrons as shown in shorthand notation

Paramagnetic - 1 unpaired e^- in the π_{2p} (compared to 0 unpaired e^- in C_2, which means C_2 doesn't interact with or is weakly repelled by a magnetic field).

b) NO^- (use the MO configuration for O_2) # e^- = 7 + 8 + 1 = 16 (# valence electrons)

$(\sigma_{1s})^2(\sigma_{1s}*)^2(\sigma_{2s})^2(\sigma_{2s}*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}*)^2(\sigma_{2p}*)^0$ (don't need empty orbitals)

$KK(\sigma_{2s})^2(\sigma_{2s}*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}*)^2$ shorthand

(replace both σ_{1s} with K and left off empty orbitals - not asked for)

B.O. = ½ (# bonding electrons − # anti-bonding electrons)

= ½ (10 − 6) = **2** (smaller B.O. than NO, double bond)

Can use just the valence electrons as shown in shorthand notation

Paramagnetic - 2 unpaired e^- in the $\pi_{2p}*$ (compared to 1 unpaired e^- in NO, which means NO^- interacts more strongly with a magnetic field).