Chem 1515
Problem Set \#1
Spring 2001

Name $\qquad$
TA Name $\qquad$
Lab Section \# $\qquad$
ALL work must be shown to receive full credit. . Due at the beginning of lecture on Wednesday, January 24, 2001.

PS1.1. Complete the following table

| Geometry | Compound | Number of bonding groups on central atom | Number of nonbonding pairs on central atom | Name of the molecular geometry | $\begin{gathered} \text { Bond } \\ \text { Angle(s) }) \\ \hline \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{NO}_{2}{ }^{-}$ | 2 | 1 | bent | $\sim 120{ }^{\circ}$ |
|  | $\mathrm{CH}_{4}$ | 4 | 0 | tetrahedral | $109.5^{\circ}$ |
|  | HCN | 2 | 0 | linear | $180^{\circ}$ |
|  | $\mathrm{SF}_{4}$ | 4 | 1 | seesaw | $90^{\circ}$ $\sim 119^{\circ}$ $\sim 178^{\circ}$, |
|  | $\mathrm{XeF}_{4}$ | 4 | 2 | square planar | $90^{\circ}$ |

PS1.2. Use simple structure and bonding models to account for each of the following.
a) The $\mathrm{H}-\mathrm{N}-\mathrm{H}$ bond angle is $107.5^{\circ}$ in $\mathrm{NH}_{3}$.

Ammonia has three bonding pairs of electrons and one nonbonding pair of electrons. The electron-pair geometry about a central atom with four bonding pairs of electrons and no lone pairs is tetrahedral with bond angles of $109.5^{\circ}$. The replacement of one bonding pair with a nonbonding pair, decreases the $\mathrm{H}-\mathrm{N}-\mathrm{H}$ bond angle to $107^{\circ}$. The decrease in the bond angle is due to the nonbonding electron pair-bonding electron pair repulsions. The nonbonding pair of electrons occupy a larger volume of space compared to the bonding pair of electrons because a lone pair is associated with only one nucleus while a bonding pair is associated with two nuclei. The attraction to two nuclei dimenishes the volume of space the electron pair occupies.

PS1.2. (CONTINUED)
b) The $\mathrm{I}_{3}$ - ion is linear.

The central iodine atom has five pairs of electrons. The electron geometry is trigonal bipyramidal. Of the five pair of electrons, two are bonding and three are nonbonding. To minimize the bonding electron pair-nonbonding electron pair repulsions, the nonbonding electron pairs occupy the trigonal plane (equatorial) and the bonding electron pairs are axial. The molecular geometry is linear.

PS1.3. Which of the molecules list in PS1.1. above are polar and which are nonpolar? In each case support your answer with a brief explanation.

| Geometry | Compound | Polarity |
| :---: | :---: | :---: |
|  | polar |  |

PS1.4. Indicate the hybridization on the central atom for each of molecules in PS1.1. above.

| Geometry | Compound | Hybrization |
| :---: | :---: | :---: |
|  | $\mathbf{N p}^{2}$ |  |

PS1.5. Consider the Lewis structure for glycine

(a) What are the approximate bond angles about each of the two carbon atoms, and what are the hybridization of the orbitals on each of them?
(b) What are the hybridization of the orbitals on each of the two oxygen atoms and the nitrogen atom, and what are the approximate bond angles at the nitrogen?
(c) What is the total number of $\sigma$ bonds in the entire molecule, and the total number of $\pi$ bonds?

a) Carbon atom $\mathrm{C}_{1}$ has bond angles of $109.5^{\circ}$ and $\mathrm{sp}^{3}$ hybridization. The $\mathrm{C}_{2}$ has bond angles of $120^{\circ}$ and $\mathrm{sp}^{2}$ hybridization.
b) Nitrogen atom $\mathbf{N}_{1}$ bond angles are approximately $107^{\circ}$.
c) There are nine sigma bonds and 1 pi bond.

PS1.6. Problem 11.47 on page 419 and 420 in Silberberg. Be sure to re-draw the structure of tryptophan below then answer each part of the question.



PS1.7. Indicate the atomic and/or hybrid orbitals on each atom in the following molecules that are involved in forming the covalent bond.
a) $\mathrm{H}-\mathrm{F}$

The hydrogen atom has a valence electron in a $1 s$ orbital, the fluorine atom has a valence electron in a $2 p$ orbital. So the overlap is between a $1 s$ orbital on $H$ and a $2 p$ orbital on fluorine.
b) $\mathrm{F}_{2}$

Both fluorine atoms have a valence electron in a $2 p$ orbital. So the overlap is between a $2 p$ orbital on each fluorine atom.
c)
: $\mathrm{C} \equiv \mathrm{O}$ :
The carbon atom is $s p$ hybridized. The oxgen atom forms a sigma bond with one of its $2 p$ orbitals and an $s p$ hybrid orbital on carbon. Two pi bonds are formed with the remaining $2 p$ orbitals from the carbon and oxygen atoms. Or the oxygen atom can be thought of as $s p$ hybridized, again with two $2 p$ orbitals forming $\pi$ bonds and an $s p$ hybrid orbital overlapping with the $s p$ hybrid orbital on the carbon. The lon pair on the oxygen would occupy an $s p$ hybrid orbital.

