Names: _____

Worksheet: The Structure of Molecules II
Molecular Modeling / WebMO

Using a browser that has the latest Java version enabled. (Some browser versions will not work such as some versions of Explorer.) Newer versions of Safari, Mozilla and Firefox will work. The browser must have Java enabled.

1. Access Web MO by going to: *http://butane.cabrillo.edu/*
2. Click on the Diablo Valley College link.
3. Enter your last name in the Username box using all lower case letters without a first name nor any initials. *(NOTE: See Dr. R. in the event that another Chem 121 student has the same last name as you.)*
4. Use your first name in all lower case letters as your password for your first time login and then change the password to one of your own choosing.
5. The steps used to build a molecule, *sulfur tetrafluoride,* will be demonstrated. *(Be sure to take notes.)* In a partnership of 2 to 4 per group, select two to four of the molecules from the left column below depending on how many partners you have. Build the molecules using the periodic table in the side bar menu as in the demo, close Builder and submit the job with the modeling criteria in the directions. Reload the page and from the Job output find the appropriate data for your molcule, complete the following table, and compare to the noted *jmol* molecule, which has the same molecular shape and is correctly modeled.

Reference Molecules for comparison; *SEE: http://chemconnections.org/VSEPR-jmol/*

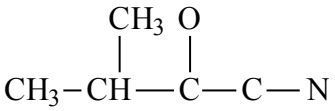
	Molecular Shape	Orbital hybridization	Bond length (nm)	Bond $\angle^{o}$	Compared Bond lengths & bond $\angle^{o}$
BH_3					vs. BF_3
H_2S					vs. H_2O
$AsCl_5$					vs. NH_3

	Molecular Shape	Orbital hybridization	Bond length (nm)	Bond $\angle^{o}$	Compare Bond lengths & $\angle^{o}$
SeO_2					vs. SO_2
CCl_4					vs. CCl_4
$BrCl_3$					vs. ClF_3
ICl_5					vs. ClF_5
SCl_6					vs. SF_6

6. Consider three molecules – A, B, C. Molecule A has a hybridization of sp^3. Molecule B has two more effective pairs (electron pairs around the central atom) than molecule A. Molecule C consists of two atoms: one σ bond and two π bonds. Give the molecular structure, hybridization, bond angles, and an example for each molecule.

	Molecule A	**Molecule B**	**Molecule C**
Molecular Structure			
Hybridization			
Bond Angles			
Example			

7. Complete the Lewis structure for the following molecule:

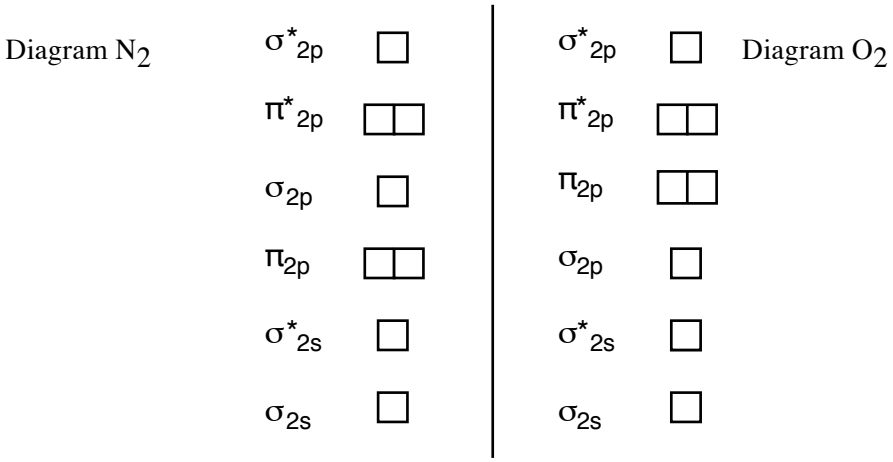


This molecule has _____ sigma and _____ pi bonds.

8. Circle any of the following statements that is incorrect.
   - I. The hybridization of boron in BF_3 is sp^2.
   - II. The molecule XeF_4 is nonpolar.
   - III. The bond order of N_2 is three.
   - IV. The molecule HCN has two pi bonds and two sigma bonds.

9. The electron configuration of a particular diatomic species is $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^4$. What is the bond order for this species?

10. General energy-level molecular orbital diagrams for two second-period homonuclear diatomic molecules are given below. Complete the energy levels using arrows for N_2 and O_2.



Determine whether each molecule is paramagnetic or diamagnetic. Explain your reasoning.

11. Circle any of the molecular orbital descriptions of CO that are correct:
   a) The highest energy electrons occupy antibonding orbitals.
   b) Six molecular orbitals contain electrons.
   c) There are two unpaired electrons.
   d) The bond order is 3.