Name:________________________ Exp #5 Computer Molecular Modeling Report Worksheets

Partner:_______________________ Fall 2014 CH145

Data/sketches	**HCl**	**H_2**	**NaH**	**O_2**	**NO**
sketch of molecule including dipole					
electronic energy RHF or UHF					
dipole moment value					
partial charges	H: Cl:	H: H:	Na: H:	O: O:	N: O:
bond length					
electron density surface sketch (=bond density)				*X*	*X*
electrostatic potential surface sketch				*X*	*X*

Experiment# 9 Computer Molecular Modeling

Data/sketches	**O_2**	**NO**
bond order		
HOMO sketch & Identity of type of bond (σ, σ*, π or π*)		
LUMO sketch & Identity of type of bond (σ, σ*, π or π*)		

O_3 Bond Orders electronic energy ___________________ bond angle _________________° (near 120°)

	O atom 1 (center atom)	O atom 2
O atom 2		*X*
O atom 3		(2 and 3 terminal atoms)

Reminder- you may have worked with a partner to obtain this data and these sketches but your responses to the following questions should be in your own words.

<u>Laboratory Report Questions for Part I:</u>

1. Consider the electronegativities of H, Cl, and Na atoms. Look at your computer model **bond density** sketches for H_2, HCl, and NaH. Do the electronegativity differences between the atoms in H_2, HCl, and NaH correspond to the ionic/covalent character of the bonds as indicated by these bond densities? (How do the bond density sketches compare to your answers of pre-lab question #1?)

2. Look at your pre-lab Lewis dot structures of H_2, HCl, and NaH. Sketch those here. Include any applicable dipole. Do the electronegativity differences between the atoms in H_2, HCl, and NaH correspond to computer model calculated **bond polarities** (as indicated by the electrostatic potential surfaces, the dipole moments, and the partial charges)?

Laboratory Report Questions for Part II:

3. Look at your pre-lab Lewis dot structure of O_2 . Sketch it here:
Draw the MO diagram of O_2 here:

4. What type of atomic orbitals form the HOMO of O_2? (*choose from s, or p along the bond direction, or p perpendicular to the bond direction*)
   What type of atomic orbitals form the LUMO of O_2? (*choose from s, or p along the bond direction, or p perpendicular to the bond direction*)

5. Is the HOMO of O_2 sigma or pi, bonding or anti-bonding?____________
   Is the LUMO of O_2 sigma or pi, bonding or anti-bonding?____________

6. Write the bond order of O_2 for your Lewis dot structure here:______.

7. Calculate the bond order of O_2 for your MO diagram here:__________________________

8. Compare the three bond orders (Lewis dot structure, MO diagram, computer model calculated). Explain any differences.

9. Look at your pre-lab Lewis dot structure of NO. Draw it here:
Draw the MO diagram of NO here (see textbook):

10. What type of atomic orbital forms the HOMO of NO? (*choose from s, or p along the bond direction, or p perpendicular to the bond direction*)
What type of atomic orbital forms the LUMO of NO? (*choose from s, or p along the bond direction, or p perpendicular to the bond direction*)

11. Is the HOMO of NO sigma or pi, bonding or anti-bonding?____________
Is the LUMO of NO sigma or pi, bonding or anti-bonding?____________

12. Write the bond order of NO for your Lewis Dot Structure here:______.

13. Calculate the bond order of NO for your MO diagram here:__________________________

14. Compare the three bond orders (Lewis dot structure, MO diagram, computer model calculated). Explain any differences.

Comparison of O_2 and NO computational models:
15. Explain why there is a difference in bond length between O_2 and NO. Use your molecular orbital diagrams and the results of the computations as a basis for your answer.

Electronic Structure of Ozone
16. Compare the computer model bond orders for ozone to the Lewis Dot Structure bond orders. Are the bonds to the central atom equivalent?

17. Consider the bond order between the terminal atoms, atoms 2 and 3. Draw the resonance structure that has a bond between atoms 2 and 3. Does this cyclic resonance structure contribute significantly to the electronic structure of ozone? How do you know? (The point of this question is to show that many different types of atomic orbital overlaps contribute to bonding, and that Lewis structures are greatly simplified representations of molecular structures.)