

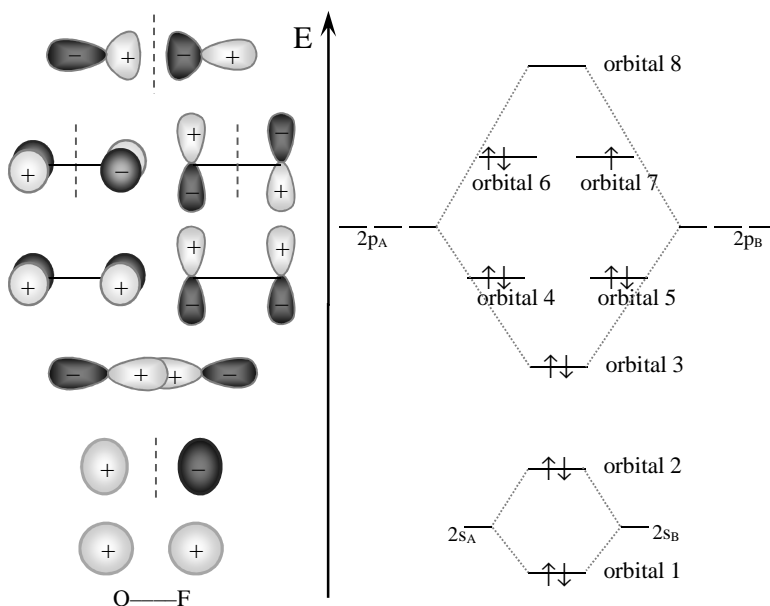
**Prelab Questions--Experiment 5: Molecular Modeling II: Molecular Orbital Theory**

**Everyone answers a, b, and c.**

- (a). Predict the bond polarity for HCl, NaH, and NO and from electronegativity differences. How covalent or ionic are these bonds? (*choose from: purely covalent, polar covalent, roughly 50% covalent, mostly ionic, purely ionic*). Remember that a difference of electronegativity of 1.7 roughly corresponds to 50% ionic. [We will use this answer in Part I of the lab.]
- (b). Draw the Lewis Dot structures for O<sub>2</sub>, NO, and O<sub>3</sub>. Draw both resonance forms for O<sub>3</sub>. [We will use this answer in Part II.]
- (c). Using qualitative molecular orbital theory, predict the highest occupied molecular orbital, HOMO, and lowest unoccupied molecular orbital, LUMO, for NO.

Answer **one** (1) of the following questions, based on the last digit of your student ID number.  
 ID ending in: 0 or 1: d      2 or 3: e      4 or 5: f      6 or 7: g      8 or 9: h

The questions are based on the following molecular orbital diagram.



ID ending in 0 or 1

- (d). Is orbital 2:  $\sigma$  or  $\pi$ ?      Is orbital 2: bonding or anti-bonding?

ID ending in 2 or 3

- (e). Which orbital corresponds to the highest occupied molecular orbital, HOMO? \_\_\_\_\_

ID ending in 4 or 5

- (f). The  $\pi$ -anti-bonding orbitals are orbitals \_\_\_\_\_

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*ID ending in 6 or 7*

(g). Is orbital 4:  $\sigma$  or  $\pi$ ?      Is orbital 4: bonding or anti-bonding?

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*ID ending in 8 or 9*

(h). The filling for the diagram is for the neutral OF diatomic molecule. What is the qualitative bond order based on this MO filling? \_\_\_\_\_

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\* The student ID number is the 6-digit number on the front of your ID card at the right-hand side