

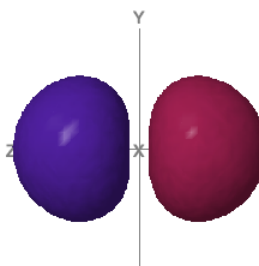
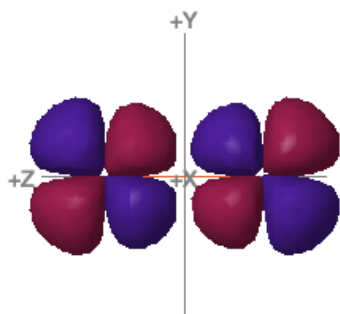
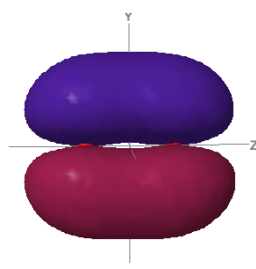
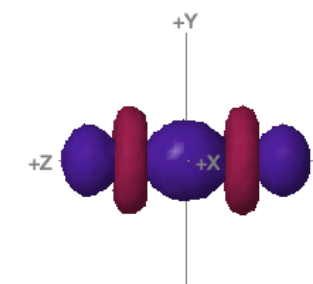
1. (15 pts.) In order to form a MO from AO's three things need to be true about the AO's. Those three things are...

2. (10 pts.) In a diatomic molecule, a $2p_x$ orbital does not have the correct symmetry to interact with a $2p_z$ orbital to form a molecular orbital. Draw the interaction between a $2p_x$ and $2p_z$ orbital and explain why this pair of orbitals cannot be used to make a molecular orbital.

3. (20 pts.) Draw a representations of the following molecular orbitals on a diatomic molecule

a. a π bonding orbital formed from two d orbitals	b. a π bonding orbital formed from two p orbitals
c. a σ bonding orbital formed from two p orbitals	d. a σ anti-bonding orbital formed from two s orbitals

4. (30 pts) Label the following MO's as bonding or anti-bonding; σ , π , or δ symmetry; and list the two atomic orbitals they are formed from. The two atoms are on the z axis equidistant from the origin.



1. _____

2. _____

3. _____

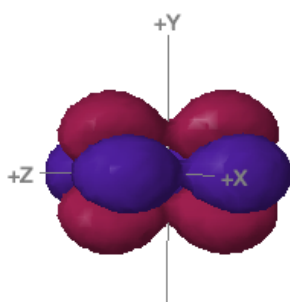
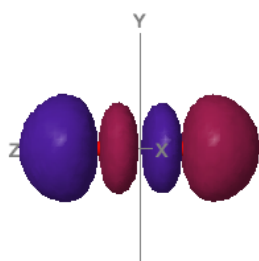
4. _____

5. _____

6. _____

7. _____

8. _____



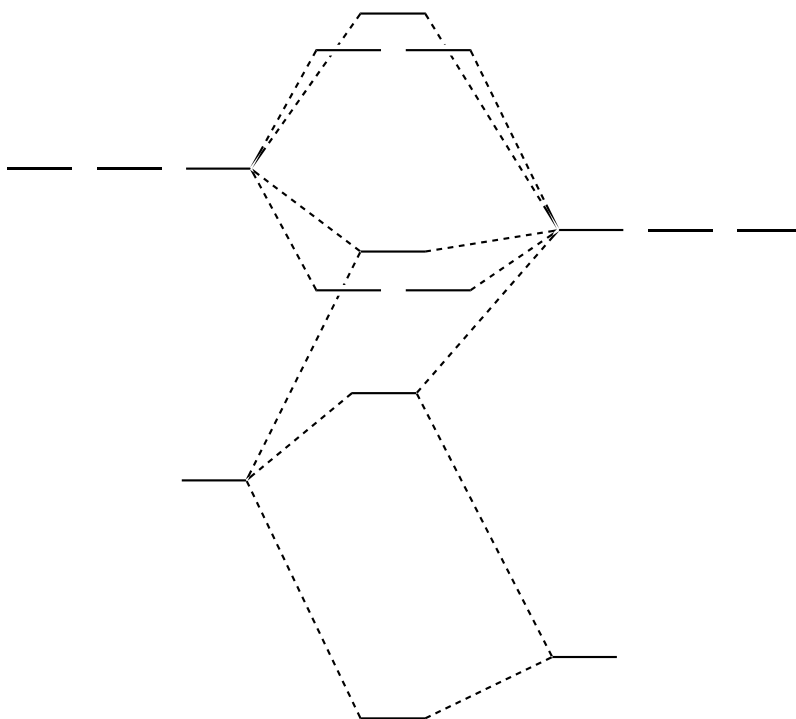
5. An incomplete MO diagram for NO is provided.

a. (4 pts.) Label the orbitals that belong to the N atom and the O atom.

b. (14 pts.) Complete the diagram by labeling the AO's, labeling the MO's (σ , π , σ^* , π^* , u and g), and adding the appropriate number of e^- 's to the orbitals.

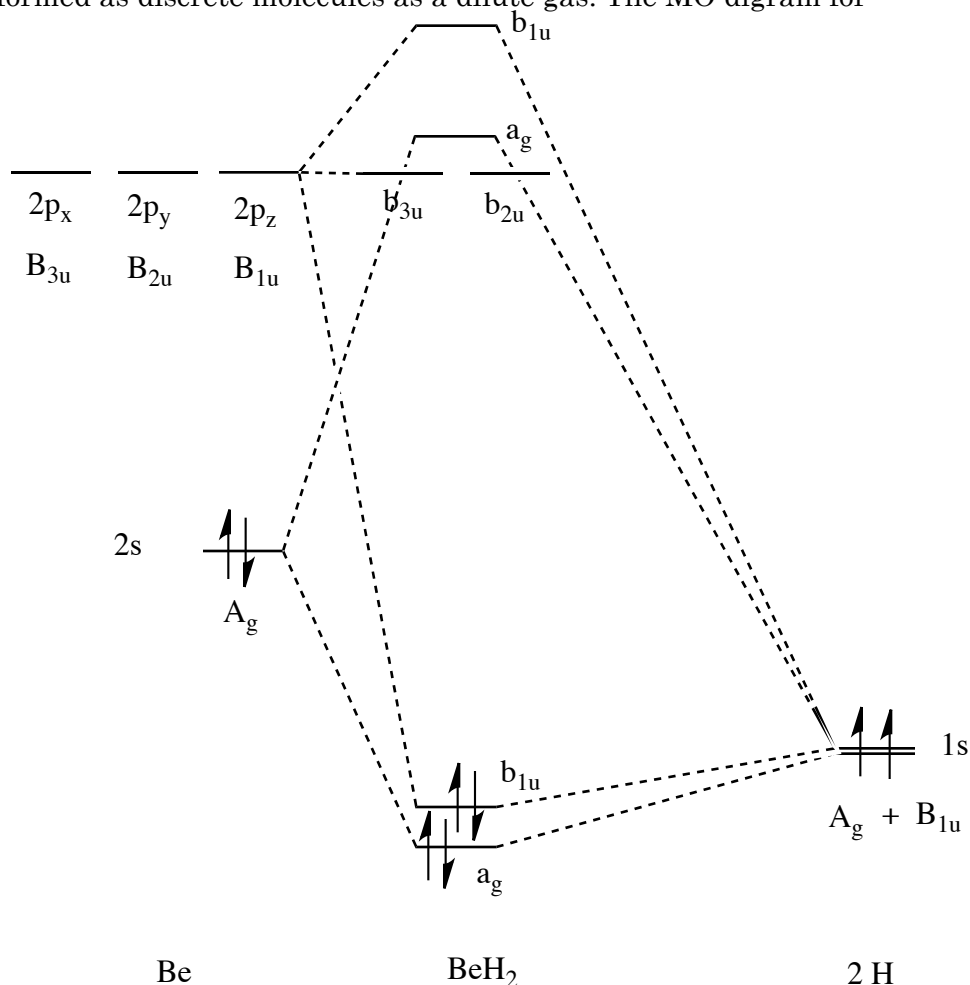
c. (6 pts.) If an electron is donated to the NO, to which orbital would the e^- be added?

f. (6 pts.) Would you expect the bond between the atoms to weaken if an electron was removed from the molecule? Explain.



6. (20 pts) Alkaline earth hydrides with the formula MH_2 (BeH_2 , MgH_2 , CaH_2) typically exist as network solids, but BeH_2 can be formed as discrete molecules as a dilute gas. The MO diagram for BeH_2 is drawn below.

a. Sketch the lower energy b_{1u} molecular orbital, which is formed from the Be $2p_z$ and the H atoms' B_{1u} symmetry SALC.



7. a. (10 pts.) What is the acronym HOMO an abbreviation for?

b. (10 pts.) What is the acronym LUMO an abbreviation for?

8. (40 pts.) Draw an MO diagram for H_2S . (a. 9 pts.) Determine the point group for H_2S . (b. 9 pts.) Determine the symmetry (the irreducible representations) of the $3s$ and $3p$ orbitals on S. (c. 9 pts.) Determine the symmetry of the group orbitals formed from the two H atom $1s$ orbitals. (d. 9 pts.) Sketch an MO diagram clearly indicating, like the one above, which orbitals are interacting. Remember to label your orbitals: use orbital names and symmetry labels for the atomic orbitals, and use symmetry labels for the molecular orbitals. (e. 4 pts.) Label the HOMO and the LUMO. The energies for the S atom's $3s$ and $3p$ orbitals are -22.7 and -11.6 eV respectively, and the energy for the H atom's $1s$ orbital is -13.6 eV.

- b. Sketch the lower energy a_g molecular orbital, which is formed from the Be 2s orbital and the H atoms' A_g symmetry SALC.