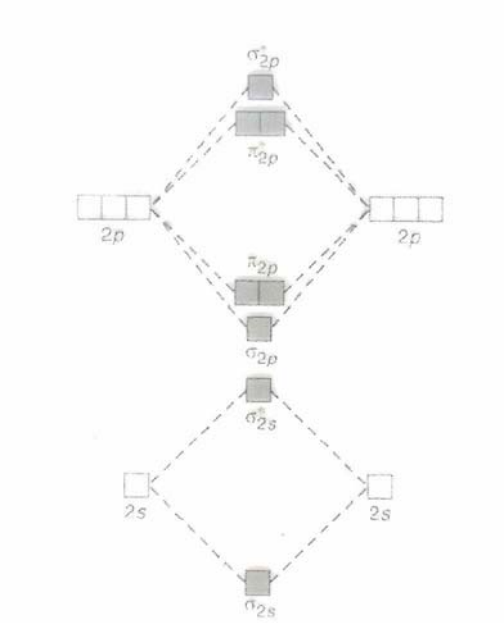
1.



Complete an MO diagram for Ne_2, give the bond order and state if the molecule is stable and why or why not?

BO = 0, molecule is not stable, no reason for bond to form. "Tree" should be filled with electron pairs.

2. One can safely assume that the 3*s*- and 3*p*-orbitals will form molecular orbitals similar to those formed when 2*s*- and 2*p*-orbitals interact. According to molecular orbital theory, what will be the bond order for the Cl_2^+ ion?

Ans: 1.5

3. The nitrosonium ion, NO^+, forms a number of interesting complexes with nickel, cobalt, and iron. According to molecular orbital theory, which of the following statements about NO^+ is correct?
   A. NO^+ has a bond order of 2 and is paramagnetic.
   B. NO^+ has a bond order of 2 and is diamagnetic.
   C. NO^+ has a bond order of 3 and is paramagnetic.
   D. NO^+ has a bond order of 3 and is diamagnetic.

Ans: D

: N ≡ O : BO = 3 Put 14 electrons into "tree" and you get BO = 3 and a diamagnetic molecule.

4. a. In the context of valence bond theory, explain the difference in geometry between a σ and a π bond. Use a real molecule to illustrate your answer.
   b. What two important differences are there in the properties of σ and π bonds, in terms of how they affect the structure and reactivity of molecules?

   a. A σ bond has its region of highest electron density between the bonded atoms, along the axis joining them. A π bond has two regions of overlap, between the atoms but above and below the axis joining them.

   b. A σ bond is stronger than a π bond. There is free rotation about a σ bond but not about a π bond, giving rise to the possibility of geometrical isomers in the latter case.

5 In the context of molecular orbital (MO) theory, explain how atomic *p* orbitals can give rise to:
   a. a σ MO
   b. a π MO

   a. A σ MO arises when atomic *p* orbitals which are directed towards each other, are combined.
   b. A π MO arises from the combination of atomic *p* orbitals which lie parallel to each other, perpendicular to the internuclear axis.

6. Explain what is meant by the term "bond order" and describe how it can be calculated using the information in a molecular orbital energy level diagram.

   The bond order in MO theory is the net number of bonds, where a pair of electrons in a bonding MO constitutes a bond and a pair in an antibonding MO constitutes an antibond. It is equal to the total number of electrons in bonding MOs minus the total number in antibonding MOs, divided by two.

Key

CHM 2045 Fall 08 Dr. Mitchell Quiz # 4
Show all work, partial credit will be given.
Answers only receive no credit! Points foe each question is indicated.
Total 30 points.

$B\emptyset \; \frac{10-10}{2} = \emptyset$

$BO = \emptyset$

1.

10e Ne

Ne 10e

π_{2p} π_{2p} } σ_{1s}

(5 points) Complete an MO diagram for Ne_2, give the bond order and state if the molecule is stable and why or why not?

$BO = \emptyset$

NOT STABLE

NO REASON FOR BOND TO FORM

π_{2p} π_{2p} π^*_{2p}
π_{2p}
σ_{2p}
π_{2p}
σ^*_{2s}
π_{2s} σ_{2s}

$\frac{6-3}{2} = \frac{3}{2} = 1.5$

Cl_2^{+1} $BO = 1.5$

2. (5 points) One can safely assume that the 3*s*- and 3*p*-orbitals will form molecular orbitals similar to those formed when 2*s*- and 2*p*-orbitals interact. According to molecular orbital theory, what will be the bond order for the Cl_2^+ ion?

BO

MO DIAGRAM

$17 + 16 = 33$e

20e $= BO$ of $\emptyset$

USING "TRUE" MODEL $\frac{6-3}{2} = 1.5$

3. **(5 points) The nitrosonium ion, NO^+, forms a number of interesting complexes with nickel, cobalt, and iron. According to molecular orbital theory, which of the following statements about NO^+ is correct?**

A. **NO^+ has a bond order of 2 and is paramagnetic.**
B. **NO^+ has a bond order of 2 and is diamagnetic.**
C. **NO^+ has a bond order of 3 and is paramagnetic.**
D. **NO^+ has a bond order of 3 and is diamagnetic.**

PUT 14 ⓔ IN "TRAP"
ABOVE BO=3
ALL PAIRED ∴ DIAMAGNETIC