

## HW10 - MO Theory

1 1 point

What is the expected bond order for the diatomic species  $B_2$  ?

- 1  
 4  
 0  
 2  
 3

2 1 point

Consider the molecule  $B_2$  (explored above in question #1). What is the magnetism and number of unpaired electrons in  $B_2$ ?

- diamagnetic, 0  
 paramagnetic, 2  
 paramagnetic, 1  
 diamagnetic, 2

3 1 point

According to molecular orbital theory, which of the following is NOT predicted to exist?

- $He^{2-}$   
 He  
 All are predicted to exist.  
  $He^{2+}$   
  $He_2$

4 1 point

$N_2$  has a bond order of 3 and  $O_2$  has a bond order of 2. Based on this information, choose the response that best completes the following sentence:  $N_2$  is (less, more) stable than  $O_2$ , and has a (larger, shorter) bond length and a (higher, lower) bond energy.

- less, shorter, lower  
 more, shorter, higher  
 less, longer, lower  
 more, shorter, lower

5 1 point

Which of the following species possesses a delocalized bond?

- $NCl_3$   
 No molecule given here possesses a delocalized bond.  
  $H_2O$   
  $H_2S$   
  $NO_3^-$

6 1 point

Which of the following statements concerning molecular orbital theory is true?

1. Bonding orbitals are lower in energy than their corresponding anti-bonding orbitals.
2. If a molecule has an odd number of electrons, then it is paramagnetic.
3. The MO diagrams for  $O_2$ ,  $F_2$ ,  $Ne_2$  are NOT filled using the Aufbau principle.

- 1 and 2       1, 2, and 3  
 1 and 3       2 and 3  
 1 only       2 only

7 1 point

Which of the following statements concerning molecular orbital theory is/are true?

1. Bonding orbitals are equal in energy to their corresponding anti-bonding orbitals.
2. Adding electrons to anti-bonding orbitals destabilizes molecules.
3. Unlike when we fill atomic orbitals, we DON'T use Hund's Rule to fill molecular orbitals.

- 1, 2, and 3  
 1 only  
 2 only  
 1 and 3  
 2 and 3  
 3 only

8 1 point

Which of the following statements is true about a molecule with a bond order of one?

- The molecule has a single bond.  
 The molecule has no electrons in antibonding orbitals.  
 The molecule is as stable as molecules with bond orders of two and three.  
 Two side-by-side p orbitals combine to form pi bond and pi antibond orbitals; therefore, the bond order is 1.

9 1 point

Which of the following must be observed when filling a molecular orbital energy diagram?

- Aufbau Principle, Conservation of Matter and Energy, and Planck's Law  
 Hund's Rule, Pauli Exclusion Principle, and Dalton's Law  
 Aufbau Principle, Hund's Rule, and Pauli Exclusion Principle  
 Aufbau Principle, Hund's Rule, and Graham's Law

10 1 point

Will  $H_2^+$  be more or less stable than  $H_2$  and why?

- more stable;  $H_2^+$  has one less electron in bonding orbitals  
 more stable;  $H_2^+$  has one less electron in antibonding orbitals  
 less stable;  $H_2^+$  has one less electron in antibonding orbitals  
 less stable;  $H_2^+$  has one less electron in bonding orbitals

11 1 point

A chemist has synthesized two new dyes based on the molecular structure of plant-based dyes. The lowest energy absorption line for the first dye is light in the visible region at 530 nm. The lowest energy absorption line for the second dye is light in the visible region at 645 nm. Based on this evidence, which molecule has the larger HOMO-LUMO gap?

- The dye that absorbs at 530 nm.  
 The dye that absorbs at 645 nm.  
 The gap is the same as both dyes absorb light in the visible region.  
 There is not enough information given to answer the question.

12 1 point

An antibonding orbital is formed when...

- an s-orbital overlaps a p-orbital.  
 a free electron is present in the molecule.  
 the overlap of the corresponding atomic orbitals leads to destructive interference.  
 a  $p_x$ -orbital overlaps a  $p_z$ -orbital.

13 1 point

Which of the following are important contributions that MO theory makes to chemistry?

1. The ability to use MO theory with a computer to calculate the minimum energy geometry of a molecule.
2. The ability to predict the energy at which a molecule will absorb light.
3. The ability to predict whether or not a molecule should be paramagnetic or diamagnetic.

- 1 only  
 2 only  
 2 and 3  
 1, 2, and 3  
 1 and 2  
 1 and 3  
 3 only