HW10 - MO Theory

Question 1 2 pts

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

- 1
- 2
- 4
- 3
- 0

Question 2 3 pts

Consider the molecule B_2 (explored above in question #4). What is the magnetism and number of unpaired electrons in B_2?

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

Question 3 2 pts

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

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

Question 4 3 pts

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.

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

Question 5 2 pts

Which of the following species possesses a delocalized bond?

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

Question 6 2 pts

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

Question 7 2 pts

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

Question 8 2 pts

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

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

Question 9 2 pts

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

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

Question 10 2 pts

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

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

Question 11 3 pts

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

Question 12 3 pts

An antibonding orbital is formed when...

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

Question 13 2 pts

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.

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