I. Multiple Choice

1. Which molecule is correctly matched with its shape as predicted by VSEPR theory?
   (A) PCl₃ trigonal pyramidal
   (B) OF₂ linear
   (C) ClF₃ trigonal planar
   (D) SF₆ hexagonal

2. Which statement about the molecular orbitals in a molecule is correct?
   (A) No molecular orbital may have a net overlap with any other molecular orbital.
   (B) Each molecular orbital must have a different number of nodes than every other molecular orbital.
   (C) The number of molecular orbitals is equal to half the number of atomic orbitals of the atoms that make up the molecule.
   (D) The lowest-energy molecular orbitals are the most bonding in character and the highest-energy molecular orbitals are the most antibonding in character.

3. Allene has the structure H₂C=C=CH₂. What is the best description of the geometry of allene?
   (A) Linear     All in the same plane
   (B) Linear     In two perpendicular planes
   (C) Bent       All in the same plane
   (D) Bent       In two perpendicular planes

4. What is the bond order of carbon monoxide, CO?
   (A) 1.5 (B) 2.0 (C) 2.5 (D) 3.0

5. Which statements about the best Lewis structure of the fulminate ion, CNO⁻, are correct? (C is central atom)
   I. The nitrogen atom has a positive formal charge.
   II. The nitrogen atom has a lone pair of electrons.
   (A) I only (B) II only (C) Both I and II (D) Neither I nor II

6. Which species contains three sigma bonds and one pi bond?
   (A) PF₃ (B) NH₄⁺ (C) C₂H₂ (D) CO₃²⁻

7. According to molecular orbital theory, removing an electron from molecular oxygen, O₂, to form the dioxygenyl cation, O₂⁺, causes what changes in the bond length and in the number of unpaired electrons?
   Bond length      Number of unpaired electrons
   (A) Increase     Increase
   (B) Increase     Decrease
   (C) Decrease     Increase
   (D) Decrease     Decrease

8. Which of the following molecules has a dipole moment of zero?
   (A) HCN     (B) CH₂Cl₂
   (C) SO₂     (D) CO₂

9. Formamide has the structure HC(O)NH₂. Which atoms in formamide have a trigonal planar geometry?
   (A) C only     (B) N only
   (C) Both C and N (D) None of them
10. Determine the electron geometry of NCl₃.  
   A. tetrahedral  
   B. linear  
   C. trigonal planar  
   D. trigonal bipyramidal  
   E. octahedral

11. Give the approximate bond angle for a molecule with an octahedral shape.  
   A. 109.5°  
   B. 180°  
   C. 120°  
   D. 105°  
   E. 90°

12. Which of the following statements is TRUE?  
   A. The total number of molecular orbitals formed doesn't always equal the number of atomic orbitals in the set.  
   B. A bond order of 0 represents a stable chemical bond.  
   C. When two atomic orbitals come together to form two molecular orbitals, one molecular orbital will be lower in energy than the separate atomic orbitals and one molecular orbital will be higher in energy than the separate atomic orbitals.  
   D. Electrons placed in antibonding orbitals stabilize the ion/molecule.  
   E. All of the above are true.

13. Use molecular orbital theory to determine which of the following are paramagnetic.  
   A. O₂²⁻  
   B. Ne₂²⁺  
   C. O₂²⁺  
   D. F₂²⁺  
   E. None of the above are paramagnetic.

14. When two atomic orbitals overlap in phase, all of the following occur except:  
   A. constructive interference occurs  
   B. a bonding molecular orbital is produced  
   C. the energy of the orbital is always higher and therefore more stable  
   D. the orbitals are added, not subtracted

15. According to valence bond theory, the triple bond in ethyne (acetylene, C₂H₂) consists of  
   A. three σ bonds and no π bonds.  
   B. two σ bonds and one π bond.  
   C. one σ bond and two π bonds.  
   D. no σ bonds and three π bonds.  
   E. none of these choices is correct.

16. Describe a pi bond.  
   A. side by side overlap of p orbitals  
   B. end to end overlap of p orbitals  
   C. s orbital overlapping with the end of a p orbital  
   D. overlap of two s orbitals  
   E. end to end overlap of a p orbital with a d orbital

17. Give the hybridization for Br in BrF₅.  
   A. sp³d²  
   B. sp³d  
   C. sp³  
   D. sp²  
   E. sp

18. Use the molecular orbital energy diagram shown to determine which of the following is most stable (has highest bond order).  
   A. C₂²⁺  
   B. N₂²⁺  
   C. B₂  
   D. C₂²⁺  
   E. B₂²⁺
### II. Short Answer

1. **Best Lewis Structure**
   - A. CHCl₃
   - B. H₂CO
   - C. NH₂Cl
   - D. PO₄³⁻
   - E. SeF₅⁻

   (show all electrons and bonds) has lowest FC. Show all nonzero FCs.

<table>
<thead>
<tr>
<th>Hybridization</th>
<th>e⁻ geometry</th>
<th>Molecular geometry</th>
<th>Approx. Bond angles</th>
<th>Polar or non-polar (don't worry about ions)</th>
<th>Number of σ bonds</th>
<th>Number of π bonds</th>
<th>Total lone pairs in the entire molecule</th>
<th>Number of nonbonding electron pairs on the central atom</th>
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2. Draw the orbital overlap diagram for CH₂CH₂. Your diagram should include the type of each atomic orbital (s, p, d, sp², etc.) and whether the overlap forms a sigma or pi orbital.

3. Draw the Lewis structure and orbital overlap diagram for the HCN molecule. Then create a version of the orbital overlap diagram that is **ACTUALLY** three dimensional. Pictured below is a simple example.
4. Consider the molecule BrF₅.
   A. Draw the best Lewis structure for this molecule. Label any atoms with nonzero formal charge.
   B. Label each bond angle. As part of your answer be sure to include if it is more or less than the ideal bond angle.
   **Answers for A-E here:**
   
   C. What is the electron geometry around the bromine atom?
   D. Are the bonds in the molecule polar?
   E. This molecule is polar, which means that it has a molecular dipole. Describe or draw the molecular dipole. Make sure to make your description/drawing clear.

5. Consider the molecule CH₂F₂.
   A. Draw the best Lewis structure for this molecule.
   B. Label each bond angle.
   **Answers for A-D here:**
   
   C. Redraw the shape of the molecule (according to the exacting specifications of your instructor). Draw all dipoles.
   D. This molecule is polar, which means that it has a molecular dipole. Describe or draw the molecular dipole. Make sure to make your description/drawing clear.

6. Consider the molecule CH₂CF₂.
   A. Draw the best Lewis structure for this molecule.
   B. Label each bond angle.
   **Answers for A-D here:**
   
   C. Redraw the shape of the molecule. Draw all dipoles.
   D. This molecule is polar, which means that it has a molecular dipole. Describe or draw the molecular dipole. Make sure to make your description/drawing clear.
7. Consider the ion \( \text{SO}_4^{2-} \). Draw all 6 resonance structures. Label all nonzero formal charges.

8. The molecular orbital energy diagram for the valence orbitals of the CN molecule and the CN\(^-\) ion is shown to the right. Use this diagram to answer the following questions.
   A. Fill in all of the electrons for the CN molecule.
   B. What is the bond order in CN?
   C. What is the bond order in CN\(^-\)?
   D. Is CN\(^-\) diamagnetic, or is it paramagnetic? How can you tell?
   E. Which has the larger bond length, CN or CN\(^-\)?

9. Two p orbitals can combine to form molecular orbitals in several different ways. Draw a sketch of the overlap between these two atomic orbitals that would produce each of the following molecular orbitals.
   A. a pi bonding MO
   B. a sigma antibonding MO

10. For each of the following molecules, make a list of the molecules that are (i) polar, (ii) nonpolar and (iii) ionic.
    A. H\(_2\)O  
    B. CH\(_4\)  
    C. CH\(_3\)CH\(_2\)OH  
    D. CH\(_3\)Cl  
    E. Na\(_2\)SO\(_4\)  
    F. HCl  
    G. C\(_6\)H\(_6\)  
    H. CH\(_3\)COCH\(_3\)  
    I. CCl\(_4\)
11. Sketch the shapes of the $\sigma_{2s}$ and $\sigma_{2s}^*$ molecular orbitals formed by the overlap of two neon $2s$ atomic orbitals.

12. For each of the molecules in the list below, give the following information:

<table>
<thead>
<tr>
<th></th>
<th>A. CHF3</th>
<th>B. HNO3</th>
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<tbody>
<tr>
<td>i. Best Lewis Structure</td>
<td></td>
<td></td>
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<tr>
<td>ii. Hybridization on the C atom</td>
<td></td>
<td>ii. Hybridization on the N atom</td>
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<tr>
<td>iii. Electron geometry on the C atom</td>
<td></td>
<td>iii. Electron geometry on the N atom</td>
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<tr>
<td>iv. Approximate bond angles about the C atom</td>
<td></td>
<td>iv. Approximate bond angles around the N atom</td>
</tr>
<tr>
<td>v. Draw the shape with in and out wedges (as necessary) and <strong>dipole arrows</strong> around the C atom.</td>
<td></td>
<td>v. Draw the shape with in and out wedges (as necessary) and <strong>dipole arrows</strong> around the N atom.</td>
</tr>
<tr>
<td>vi. Is the molecule polar or nonpolar?</td>
<td></td>
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13. This problem looks at the electron geometry and hybridization of methane, CH₄.
   A. Draw methane in its proper electron geometry.
   B. What is the hybridization on the carbon atom in methane?
   C. Justify this hybridization by:
      i) drawing all of the electrons in the unhybridized carbon atom.
      ii) drawing and naming all of the energy levels for the hybridized carbon atom and then filling in all of the electrons.
14. Pictured below is the **correct** Molecular Orbital Energy Diagram for carbon monoxide, CO.

A. Place all of the electrons in the proper molecular orbitals. (4 points)

B. What is the bond order for CO? (4 points)

C. What would be the bond order for CO⁻? (2 points)

D. Would CO be paramagnetic or diamagnetic? (2 points)

15. Formal charge (FC) guidelines assume that all bonding electrons are shared evenly between the two bonded atoms. Oxidation number (ON) guidelines assume that the more electronegative atom in the bond gets all of the shared bonding electrons. Dipole theory assumes that the bonded electrons are associated more with the more electronegative atom. **Now that you understand the basis for the ON and FC guidelines, determine the oxidation number and formal charge for each atom in propane.** You will need to draw the Lewis structure of propane (twice) for your answer.

\[
\text{FC} = (\# \text{valence e}^- \text{from PT}) - [\# \text{bonds to atom} + \# \text{single e}^- \text{on atom}]
\]

\[
\text{ON} = (\# \text{valence e}^- \text{from PT}) - [\# e^- \text{assigned to atom}]
\]