LEARNING OBJECTIVES

Demonstrate an understanding of quantum theory by characterizing the wave properties of an electron.
   Multiple Choice: 1, 2

Explain how an electron’s wave function relates to its phase, its probability of being found at a particular location in space, and the shape of its orbital.
   Multiple Choice: 3

Diagram s and p atomic orbitals, along with their relative phase and orientation.
   Multiple Choice: 40

Describe how hybridized atomic orbitals can be generated from pure s and p atomic orbitals via constructive interference and destructive interference.
   Multiple Choice: 18

Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure.
   Multiple Choice: 1–13, 23, 38
   Short Answer: 5, 7, 8

Determine the hybridization and geometry for an atom in an organic functional group or molecule.
   Multiple Choice: 7, 8, 19–22
   Short Answer: 6, 15, 16

Identify the tenets and explain the importance of molecular orbital theory.
   Multiple Choice: 6, 9

Identify a molecular orbital as having either σ or π symmetry, and explain the consequence of such symmetry with respect to bond properties.
   Multiple Choice: 10, 25, 26, 28, 31
   Short Answer: 12

Identify the total number of σ and π bonds for a molecule and the orbitals that overlap to form each bond.
   Multiple Choice: 14–17, 24, 29
   Short Answer: 3, 10, 11

Construct the atomic orbital and molecular orbital picture of the bonding in a molecule.
   Short Answer: 1, 4, 9

Identify a molecule's highest occupied molecular orbital, lowest unoccupied molecular orbital, and nonbonding orbitals.
   Multiple Choice: 4, 5, 27, 30

Identify whether cis and trans configurations are possible for a given double bond.
   Multiple Choice: 32

Classify the relative configuration of an alkene within a complex molecule as cis or trans.
   Multiple Choice: 33, 34

Explain the origin of effective electronegativity for sp, sp², and sp³ atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.
MULTIPLE CHOICE

1. Boat A follows Boat B across a lake, keeping a safe distance. The waves generated by the two boats meet to create a new wave that is unusually large. What chemical concept explains the formation of the larger wave?
   a. Destructive interference occurs.
   b. Constructive interference occurs.
   c. Molecular orbital interference occurs.
   d. The Heisenberg uncertainty principle dominates.
   e. Hund’s rule plays a role.

   ANS: B  DIF: Difficult  REF: 3.1 | 3.2
   OBJ: Demonstrate an understanding of quantum theory by characterizing the wave properties of an electron.  MSC: Analyzing

2. Boat A and Boat B start on opposite sides of a lake. The boats cross the lake heading directly toward one another at equal rates of speed. Upon meeting, what happens to the waves generated by the two boats?
   a. Destructive interference occurs, and thus the waves negate each other, leaving only a ripple.
   b. Constructive interference occurs, and thus the new wave formed is larger in size.
   c. The Heisenberg uncertainty principle dominates, and thus the outcome of the meeting of the two waves is not concrete.
   d. Destructive interference occurs, forming one wave that is much larger in size.
   e. Constructive interference occurs, forming one wave that is much larger in size.

   ANS: A  DIF: Difficult  REF: 3.1 | 3.2
   OBJ: Demonstrate an understanding of quantum theory by characterizing the wave properties of an electron.  MSC: Analyzing

3. An atom’s electrons have a high probability of being found within a region of three-dimensional space defined by quantum mechanics. What term identifies this region?
   a. Electron configuration
   b. Atomic orbital
   c. Central core
   d. Nucleus
   e. Valence shell

   ANS: B  DIF: Easy  REF: 3.1 | 3.3
   OBJ: Explain how an electron’s wave function relates to its phase, its probability of being found at a particular location in space, and the shape of its orbital.  MSC: Understanding

4. What abbreviation is used to designate the molecular orbital of highest energy that is occupied with electrons?
   a. MOHE
   b. HOME
   c. HOMO
   d. HAHA
   e. LUMO

   ANS: C  DIF: Easy  REF: 3.3
   OBJ: Identify a molecule’s highest occupied molecular orbital, lowest unoccupied molecular orbital, and nonbonding orbitals.  MSC: Remembering
5. What abbreviation is used to designate the lowest-energy molecular orbital for a molecule that is
dvoid of electrons?
   a. MOLE  
   b. LUMO  
   c. LEMO  
   d. NEMO  
   e. MOWO  
ANS: B  DIF: Easy  REF: 3.3  
OBJ: Identify a molecule’s highest occupied molecular orbital, lowest unoccupied molecular
orbital, and nonbonding orbitals.  MSC: Remembering

6. Which of the following statements about molecular orbital theory are true?
I. According to MO theory, electrons are localized on specific atoms.
II. The linear combination of atomic orbitals method is used to generate molecular orbitals for
   a molecule.
III. The number of molecular orbitals created from the LCAO approach is identical to the number
   of atomic orbitals that were originally combined.
IV. Molecular orbital theory is a powerful bonding theory that accurately predicts structures of
   complex molecules.
V. The MOs generated are classified as either bonding, nonbonding, or antibonding.
   a. Only II, III, and IV are true.  
   b. Only III, IV, and V are true.  
   c. Only IV and V are true.  
   d. All choices except I are true.  
   e. All choices are true.  
ANS: D  DIF: Medium  REF: 3.3  
OBJ: Identify the tenets and explain the importance of molecular orbital theory.  
MSC: Evaluating

7. Which of the following functional groups has a lone pair residing in an sp-hybridized orbital?
   a. Amide  
   b. Alkyne  
   c. Amine  
   d. Nitrile  
   e. Ester  
ANS: D  DIF: Easy  REF: 3.3 | 3.4  
OBJ: Determine the hybridization and geometry for an atom in an organic functional group or
molecule.  
MSC: Remembering

8. Which functional group has two sp\(^2\)-hybridized oxygen atoms within its structure, yet cannot be a
H-bond donor?
   a. Amide  
   b. Alcohol  
   c. Ester  
   d. Ketone  
   e. Aldehyde  
ANS: C  DIF: Medium  REF: 3.3 | 3.4  
OBJ: Determine the hybridization and geometry for an atom in an organic functional group or
molecule.  
MSC: Applying

9. Which characteristics describe the bonding MO for the weakest individual covalent bond in ethene,
   \(\text{C}_2\text{H}_4\)?
I. The MO possesses \(\pi\) symmetry.
II. The MO possesses \(\sigma\) symmetry.
III. The MO can be called the HOMO.
IV. The MO can be called the LUMO.
V. The MO contains two electrons of opposing spin.
   a. All of the choices  
   b. I and V  
ANS: D  DIF: Medium  REF: 3.3 | 3.4  
OBJ: Determine the hybridization and geometry for an atom in an organic functional group or
molecule.  
MSC: Applying
b. II, III, and V   c. I, III, and V
ANS: E   DIF: Difficult   REF: 3.3 | 3.4

OBJ: Identify the tenets and explain the importance of molecular orbital theory.
MSC: Evaluating

10. Which two atomic orbitals overlap to form the MOs of $\sigma$ symmetry that correspond to the C—C bond in ethylene?
   a. 2$s$ and 2$p$
   b. 2$p$ and $sp^2$
   c. $sp^2$ and $sp^2$
   d. $sp^3$ and $sp^3$
   e. 2$p$ and 2$p$

ANS: C   DIF: Easy   REF: 3.3 | 3.5

OBJ: Identify a molecular orbital as having either sigma or pi symmetry, and explain the consequence of such symmetry with respect to bond properties. 
MSC: Remembering

11. Which two carbon atoms participate in the longest $\sigma$ bond?

   a. C$_1$—C$_2$
   b. C$_2$—C$_3$
   c. C$_3$—C$_4$
   d. C$_4$—C$_5$
   e. C$_7$—C$_8$

ANS: E   DIF: Easy   REF: 3.3 | 3.5

OBJ: Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure. 
MSC: Applying

12. Which two carbon atoms participate in the strongest $\sigma$ bond?

   a. C$_1$—C$_2$
   b. C$_2$—C$_3$
   c. C$_3$—C$_4$
   d. C$_4$—C$_5$
   e. C$_7$—C$_8$

ANS: A   DIF: Easy   REF: 3.3 | 3.5

OBJ: Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure. 
MSC: Applying

13. Rank the highlighted $\sigma$ bonds in order of decreasing length.
14. Recall that ethyne is H:C≡CH. Which two orbitals share electrons in one of ethylenes covalent C—H bonds?
   a. H_s and C_p
   b. H_s and C_2p
   c. H_s and C_sp
   d. H_1s and C_sp2
   e. H_1s and C_sp

   ANS: E  DIF: Easy  REF: 3.4  
   OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  MSC: Remembering

15. Which C—C bond in the molecule below is formed from overlap of two sp2-hybridized orbitals?

   a. The C_1—C_2 σ bond
   b. The C_7—C_8 σ bond
   c. The C_5—C_6 σ bond
   d. The C_4—C_5 π bond
   e. The C_4—C_5 σ bond

   ANS: E  DIF: Easy  REF: 3.4  
   OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  MSC: Understanding

16. Which C—C bond in the molecule below is formed from overlap of two 2p orbitals?

   a. The C_1—C_2 σ bond
   b. The C_1—C_2 π bond
   c. The C_3—C_4 σ bond
   d. The C_3—C_4 π bond
   e. The C_4—C_5 σ bond

   ANS: B  DIF: Medium  REF: 3.4
OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  MSC: Understanding

17. Which C—C bond in the molecule below is formed from overlap of an $sp^3$ orbital and an $sp^2$ orbital?

![Molecule diagram]

a. The $C_1—C_2 \sigma$ bond  

b. The $C_1—C_2 \pi$ bond  

c. The $C_3—C_4 \sigma$ bond  

d. The $C_3—C_4 \pi$ bond  

e. The $C_4—C_5 \sigma$ bond  

ANS: C  DIF: Medium  REF: 3.4

OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  MSC: Understanding

18. According to valence bond theory, which atomic orbitals of carbon may be hybridized to account for bonding? Why?

a. $1s$, $2s$, and $2p$ orbitals all may hybridize; these orbitals are of the same phase.

b. Only $2p$ orbitals may hybridize; the $2p$ orbital is carbon’s highest-energy atomic orbital.

c. Only $1s$ and $2s$ orbitals of carbon may hybridize; each contains electrons to share in bonding.

d. Only $2s$ and $2p$ may hybridize; these orbitals contain valence electrons used in bonding.

e. Only $2s$ orbitals may hybridize; these orbitals contain valence electrons.

ANS: D  DIF: Medium  REF: 3.4

OBJ: Describe how hybridized atomic orbitals can be generated from pure s and p atomic orbitals via constructive interference and destructive interference.  MSC: Analyzing

19. Which of the following structures contains an $sp^2$-hybridized oxygen atom because a lone pair on oxygen is delocalized via resonance?

![Structures]

a. Structure I  

b. Structure II  

c. Structures II and V  

d. Structure IV  

e. Structures I and IV  

ANS: D  DIF: Medium  REF: 3.4

OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule.  MSC: Evaluating

20. Naltrexone is an antagonist at the mu opioid receptor. What is the hybridization state and geometry of the nitrogen atom in naltrexone?
a. \(sp\) hybridized and linear geometry  
d. \(sp^3\) hybridized and trigonal planar  
b. \(sp^2\) hybridized and trigonal pyramidal  
e. \(sp^3\) hybridized and bent  
c. \(sp^3\) hybridized and trigonal pyramidal  

ANS: C DIF: Medium REF: 3.4 

OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule. 

MSC: Evaluating  

21. From left to right, identify the hybridization of the three carbon atoms in the interesting organic structure below. These interesting structures are called cumulenes.

\[
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H}
\end{array}
\begin{array}{c}
\text{C} \\
\text{C} \\
\text{H}
\end{array}
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H}
\end{array}
\]

a. \(sp^3, sp^2, sp^3\)  
d. \(sp, sp, sp^2\)  
b. \(sp^3, sp, sp^3\)  
e. \(sp^2, sp^2, sp^2\)  
c. \(sp^2, sp, sp^2\)  

ANS: C DIF: Medium REF: 3.4 | 3.10 

OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule. 

MSC: Applying  

22. What is the geometry and hybridization of the central carbon atom in the cumulene below?

\[
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H}
\end{array}
\begin{array}{c}
\text{C} \\
\text{C} \\
\text{H}
\end{array}
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H}
\end{array}
\]

a. \(sp^3\) hybridized and tetrahedral  
d. \(sp^2\) hybridized and bent  
b. \(sp^3\) hybridized and trigonal pyramidal  
e. \(sp\) hybridized and linear  
c. \(sp^2\) hybridized and trigonal planar  

ANS: E DIF: Medium REF: 3.4 | 3.10 

OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule. 

MSC: Applying  

23. Given below are 2s, 2p, \(sp, sp^2\), and \(sp^3\) orbitals, all drawn to scale and in no particular order. Which of these orbitals would carbon use for a C—O \(\pi\) bond?
24. Given below are 2s, 2p, sp, sp^2, and sp^3 orbitals, all drawn to scale and in no particular order. Which of these orbitals would carbon use in the C—O σ bond of acetone?

```
I  II  III  IV  V
```

a. I  d. IV  
b. II  e. V  
c. III

ANS: B  DIF: Difficult  REF: 3.4 | 3.11

OBJ: Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure.  MSC: Evaluating

25. Which two atomic orbitals overlap to form the MOs of σ symmetry that correspond to a C—H bond in ethylene?

```
I  II  III  IV  V
```

a. An sp^2 orbital from both C and H  
b. A 2p orbital from C and an sp^3 orbital from H  
c. A 1s orbital of H and the sp^2 orbital of C  
d. A 2s orbital of H and the sp^2 orbital of C  
e. A 2p orbital from both C and H

ANS: C  DIF: Easy  REF: 3.5 | 3.6

OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  MSC: Evaluating

26. Which two atomic orbitals overlap to form the bonding and antibonding MOs of π symmetry for ethylene, C_2H_4?

```
I  II  III  IV  V
```

a. 2s and 2p  
b. 2p and sp^2  
c. sp^2 and sp^2  
d. sp^3 and sp^3  
e. 2p and 2p

ANS: E  DIF: Easy  REF: 3.6

OBJ: Identify a molecular orbital as having either sigma or pi symmetry, and explain the consequence of such symmetry with respect to bond properties.  MSC: Understanding
27. Styrene is an important industrial chemical in the generation of various plastics. Determine how many bonding molecular orbitals are created during the LCAO process to accommodate the π electrons in styrene.

![Styrene Structure]

a. Two  
b. Four  
c. Six  
d. Eight  
e. Ten

ANS: B  
DIF: Medium  
REF: 3.6  
OBJ: Identify a molecule’s highest occupied molecular orbital, lowest unoccupied molecular orbital, and nonbonding orbitals.  
MSC: Understanding

28. How many total electrons reside in molecular orbitals of π symmetry for this molecule?

![Molecule with π symmetry]

a. Two  
b. Three  
c. Four  
d. Six  
e. Eight

ANS: D  
DIF: Easy  
REF: 3.6 | 3.7  
OBJ: Identify a molecular orbital as having either sigma or pi symmetry, and explain the consequence of such symmetry with respect to bond properties.  
MSC: Applying

29. How many π bonds are present in the molecule below?

![Molecule with π bonds]

a. Three  
b. Four  
c. Five  
d. Six  
e. Seven

ANS: D  
DIF: Medium  
REF: 3.6 | 3.8  
OBJ: Identify the total number of sigma and pi bonds for a molecule and the orbitals that overlap to form each bond.  
MSC: Understanding

30. For the given molecule, an amino alcohol, how many electrons are present in nonbonding molecular orbitals?

![Molecule with nonbonding orbitals]
a. Seven  
    b. Six  
    c. Five

ANS: B  
DIF: Medium  
REF: 3.7

OBJ: Identify a molecule’s highest occupied molecular orbital, lowest unoccupied molecular orbital, and nonbonding orbitals.  
MSC: Understanding

31. An alkene contains a double bond. Why is the C= C of an alkene rigid and unable to freely rotate?  
   a. The C= C bond is very strong, and it is impossible to break it.  
   b. The σ bond gets blocked by the hydrogen atoms.  
   c. The sp² hybrid orbitals of carbon take up too much room.  
   d. The π electrons are delocalized through the σ bonds.  
   e. The 2p orbitals of the π bond overlap above and below the C— C plane to restrict rotation.

ANS: E  
DIF: Medium  
REF: 3.9

OBJ: Identify a molecular orbital as having either sigma or pi symmetry, and explain the consequence of such symmetry with respect to bond properties.  
MSC: Understanding

32. For one or more of the following molecules, (1) two distinct configurations about the double bond are possible, and (2) the –OH and – Br are trans. Select the molecule or molecules that fit this description.

   ![Molecular structures](image)

   a. I  
   b. II  
   c. III

ANS: E  
DIF: Medium  
REF: 3.9

OBJ: Classify the relative configuration of an alkene within a complex molecule as cis or trans.  
MSC: Evaluating

33. For one or more of the following molecules, two distinct configurations about the double bond are possible, and the two alkyl substituents are trans. Select the molecule or molecules that fit this description.

   ![Molecular structures](image)

   a. I  
   b. II  
   c. III

ANS: B  
DIF: Medium  
REF: 3.9

OBJ: Classify the relative configuration of an alkene within a complex molecule as cis or trans.  
MSC: Evaluating

34. Select which of the following molecules have two distinct configurations about the double bond.
35. Rank the carbon atoms in order of increasing effective electronegativity.

a. I < II < III
d. II < I < III
c. II < III < I
e. III < II < I

ANS: E  DIF: Difficult  REF: 3.11
OBJ: Explain the origin of effective electronegativity for sp, sp2, and sp3 atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.  MSC: Evaluating

36. One of the following statements about the relationship of %s character to organic structure is false. Identify which statement is false.

a. The %s character and effective electronegativity are directly proportional to one another.
b. An sp3 orbital has greater %s character than an sp2 orbital.
c. Two orbitals with high %s character will form a stronger bond.
d. A 2s orbital has greater s character than any of the hybrid orbitals.
e. An orbital with greater %s character is smaller and more compact.

ANS: B  DIF: Medium  REF: 3.11
OBJ: Explain the origin of effective electronegativity for sp, sp2, and sp3 atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.  MSC: Understanding

37. Given below are 2s, 2p, sp, sp2, and sp3 orbitals, all drawn to scale and in no particular order. Which of these orbitals exhibits 50% s character?

a. I
d. IV
b. II
e. V
c. III
38. Given below are 2s, 2p, sp, sp², and sp³ orbitals, all drawn to scale and in no particular order. Which of these orbitals represents the hybrid orbital with the lowest effective electronegativity?

- a. I
- b. II
- c. III
- d. IV
- e. V

ANS: C  DIF: Medium  REF: 3.11

OBJ: Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure.  
MSC: Evaluating

39. Given below are 2s, 2p, sp, sp², and sp³ orbitals, all drawn to scale and in no particular order. Which of these orbitals represents the hybrid orbital with the greatest effective electronegativity?

- a. I
- b. II
- c. III
- d. IV
- e. V

ANS: C  DIF: Medium  REF: 3.11

OBJ: Explain the origin of effective electronegativity for sp, sp², and sp³ atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.  
MSC: Evaluating

40. Given below are 2s, 2p, sp, sp², and sp³ orbitals, in random order. Which of these orbitals exhibits 33% s character?

- a. I
- b. II
- c. III
- d. IV
- e. V

ANS: E  DIF: Medium  REF: 3.11
41. Rank the carbon atoms in order of increasing percent s orbital character.

- a. I < II < III
- b. I < III < II
- c. II < III < I
- d. II < I < III
- e. III < II < I

ANS: E

DIF: Difficult

REF: 3.11

OBJ: Explain the origin of effective electronegativity for sp, sp2, and sp3 atoms, and extrapolate trends related to bond strength, bond length, and orbital shape. MSC: Evaluating

SHORT ANSWER

1. Amide bonds join amino acids together to make proteins. Sketch an orbital picture of the amide functional group given below. Identify the orbitals from each atom that are used to form the $\sigma$ and $\pi$ bonds in the given amide. Which orbitals house the lone pairs on N and O?

ANS:
Remember that the lone pair on the nitrogen atom is conjugated with the $\pi$ electrons in the C=O, thus, the lone pair uses a 2$p$ orbital from nitrogen. This means that the O—C—N framework is planar due to overlapping $p$ orbitals. All C—H bonds are formed from overlap of H$1s$ and C$_{sp3}$ orbitals.

DIF: Medium

REF: 3.3 | 3.4 | 3.5

OBJ: Construct the atomic orbital and molecular orbital picture of the bonding in a molecule. MSC: Creating

2. Why is a $\sigma$ bond formed from the overlap of two $sp^2$ orbitals stronger than one formed from the end-on-end overlap of two $p$ orbitals?
Generally speaking, hybrid orbital theory documents that the use of hybrid orbitals creates stronger bonds. An \( sp^2 \)-hybridized orbital has 33% \( s \) character and greater effective electronegativity than a \( p \) orbital. Thus, stronger bonds are formed between these hybrid orbitals.

OBJ: Explain the origin of effective electronegativity for \( sp \), \( sp^2 \), and \( sp^3 \) atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.

MSC: Understanding

3. Compare the \( p \) orbital orientation and overlap needed to form a \( \sigma \) bond and a \( \pi \) bond. Using an example, create a diagram for each type of bond, and differentiate between \( \sigma \) and \( \pi \) bond characteristics.

ANS:

![Diagram of \( \sigma \) and \( \pi \) bonds]

DIF: Medium    REF: 3.3 | 3.5

4. The molecule benzene, which features a conjugated ring system, has interesting properties. In fact, extended benzene-like molecules are key features of many drug classes, including DNA intercalators.

(a) Draw an energy-based electron configuration diagram for any one carbon atom in benzene. Clearly show which orbitals are hybridized and which orbital is used for the \( \pi \) bond.

(b) Next, consider the \( \pi \) MO diagram of benzene generated via the LCAO method. Add \( \pi \) electrons to the diagram, and label each orbital as \( \pi \) bonding MO or \( \pi^* \) antibonding MO. How many total electrons reside in MOs of \( \pi \) symmetry for benzene?

ANS:
(a) Each carbon has one \( 2p \) orbital left over. This leftover \( 2p \) orbital is used for the \( \pi \) bond in which each carbon participates.
(b) There are six carbons in benzene; thus, there are six $2p$ orbitals and six $\pi$ electrons to consider. These six $\pi$ electrons are housed in three bonding MOs. There are also three antibonding MOs generated during application of the LCAO method.

![Diagram of benzene with $\pi$ MOs and $\sigma$ MOs]

**DIF:** Difficult  
**REF:** 3.3 | 3.6  
**OBJ:** Construct the atomic orbital and molecular orbital picture of the bonding in a molecule.  
**MSC:** Evaluating/Creating

5. Use your knowledge of hybridization to fill in the table below. Rank the sigma bonds labeled A, B, C, and D from strongest to weakest. Explain your answer.

<table>
<thead>
<tr>
<th>C—C $\sigma$ bond label</th>
<th>Carbon atoms in the $\sigma$ bond</th>
<th>Hybridization (fill in)</th>
<th>Which orbitals overlap to form the bond? (fill in)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Carbon 6</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Carbon 7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>Carbon 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Carbon 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>Carbon 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Carbon 3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Carbon 4</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Carbon 5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**ANS:**

The strongest bond is B; the weakest bond is D. The ranking is as follows: $B > C > A > D$. Bonds formed from orbitals with greater percent $s$ character are stronger.
C—C σ bond label | Carbon atoms in the σ bond | Hybridization | Which orbitals overlap to form the bond?
---|---|---|---
A | Carbon 6, Carbon 7 | \(sp^2\), \(sp^3\) | \(Csp^2—Csp^3\)
B | Carbon 1, Carbon 2 | \(sp\), \(sp\) | \(Csp—Csp\)
C | Carbon 2, Carbon 3 | \(sp\), \(sp^3\) | \(Csp—Csp^3\)
D | Carbon 4, Carbon 5 | \(sp^3\), \(sp^3\) | \(Csp^3—Csp^3\)

DIF: Easy  
REF: 3.4

OBJ: Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure.  
MSC: Analyzing

6. Below are two reasonable acyclic structures for ozone, \(O_3\), that differ in \(\pi\) electron delocalization. Identify the hybridization of all the oxygen atoms in ozone for each individual resonance contributor. What is the geometry of the central oxygen in each structure?

ANS:
The central oxygen has an overall positive formal charge and is bent, with \(sp^2\) hybridization. In fact, all oxygen atoms in ozone are \(sp^2\), and the \(\pi\) electrons are delocalized. In cases when the oxygen atom has a negative formal charge, the lone pair of electrons is associated with a \(2p\) orbital.

Use 18 valence electrons when drawing the structure of ozone. There are two viable Lewis structures of ozone. The structures have the same atomic positions, yet differ by the position of \(\pi\) electrons and lone pairs. Thus, the two structures are resonance structures.

DIF: Easy  
REF: 3.4

OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule.  
MSC: Analyzing

7. Bioymifi is a novel small molecule that selectively triggers programmed cell death in certain cancer cells. Identify the following structural features in Bioymifi: (a) phenyl ring, (b) a lone pair found in a \(2p\) orbital that can be delocalized three different ways, (c) an \(sp^2\)-hybridized oxygen whose lone pairs are not delocalized, (d) an \(sp^2\)-hybridized oxygen whose lone pairs are delocalized, (e) a nitrogen with bent geometry, and (f) a nitrogen with trigonal planar geometry.
8. Consider the hybrid structure below and the labeling scheme provided. Draw the most stable resonance contributor. Identify the hybridization and VSEPR geometry of each atom.

ANS:
The neutral structure shown below is most stable:

<table>
<thead>
<tr>
<th>Atom</th>
<th>Hybridization</th>
<th>VSEPR geometry</th>
</tr>
</thead>
</table>
### DIF: Medium  REF: 3.4 | 3.6

**OBJ:** Extrapolate the relationship between hybridization, bond length, and/or bond strength in an organic structure.  **MSC:** Evaluating

9. Sketch an orbital picture of ethylene, H\(_2\)C\(\equiv\)CH\(_2\), and highlight the orbitals that overlap to form each \(\sigma\) and \(\pi\) bond. Identify the orbitals from each atom that overlap to form the \(\sigma\) and \(\pi\) bonds. Why is the C—C \(\pi\) bond weaker than the C—C \(\sigma\) bond? Use orbital structure as part of your explanation.

**ANS:**
Any hydrogen–carbon \(\sigma\) bond in ethylene is formed by overlap of hydrogen’s 1\(s\) orbital and carbon’s \(sp^2\) orbital. The carbon–carbon \(\sigma\) bond is formed by overlap of two adjacent \(sp^2\) hybrid orbitals. The carbon–carbon \(\pi\) bond is formed by overlap of adjacent 2\(p\) orbitals.

The \(\pi\) bond is weaker, because the electron density of the C—C \(\pi\) bond resides above and below the internuclear axis due to side-by-side overlap of 2\(p\) orbitals. On the other hand, the electron density of the C—C \(\sigma\) bond is symmetrical about the internuclear axis where the attraction for the positively charged nuclei is greatest. The \(\sigma\) bond is therefore quite strong and significantly stronger than the \(\pi\) bond between the same two atoms.
10. Formaldehyde, CH$_2$O, is a biological preservative and the simplest aldehyde. Draw the structure of formaldehyde. Determine the number of $\sigma$ bonds, the number of $\pi$ bonds, and the number of electrons occupying nonbonding MOs for formaldehyde.

ANS:

![Structure of Formaldehyde]

- 1 C–O $\sigma$ bond
- 2 C–H $\sigma$ bonds
- 2 lone pairs in nonbonding MOs

11. Acetonitrile, C$_2$H$_3$N, is a polar aprotic solvent commonly used in organic reactions. Draw the structure of acetonitrile. Determine the number of $\sigma$ bonds, the number of $\pi$ bonds, and the number of electrons occupying nonbonding MOs for the molecule.

ANS:

![Structure of Acetonitrile]

- 5 $\sigma$ bonds
- 2 $\pi$ bonds
- 1 nonbonding pair
- 2 electrons in nonbonding MO

12. Tropyllium bromide is an ionic organic compound that is soluble in water but not in diethyl ether. What is the hybridization of the positively charged carbon in tropyllium bromide? Do you expect the carbon framework to be planar? Justify your response using an orbital diagram.

ANS:
DIF: Difficult  REF: 3.6 | 3.8
OBJ: Identify a molecular orbital as having either sigma or pi symmetry, and explain the consequence of such symmetry with respect to bond properties.  MSC: Evaluating

13. Using line structures, deduce individual resonance contributors from the resonance hybrid structure given here. Identify any lone pairs that are localized, rather than delocalized. Based on orbital hybridization theory, what orbitals accommodate these lone pairs?

ANS:

The \( \text{sp}^3 \) oxygen of the ether uses \( \text{sp}^3 \)-hybridized orbitals for the two localized lone pairs. The O of the ketone has two localized lone pairs that are accommodated by \( \text{sp}^2 \)-hybridized orbitals.

DIF: Difficult  REF: 3.6 | 3.8
OBJ: Explain the origin of effective electronegativity for sp, sp2, and sp3 atoms, and extrapolate trends related to bond strength, bond length, and orbital shape.  MSC: Evaluating/Creating

14. Tubulysin D is a peptide-based marine natural product with biological activity. Identify the following structural features of tubulysin D.
   (a) Place a box around any \( \text{sp}^3 \) nitrogen.
   (b) Star (*) any oxygen atom that has two oxygen lone pairs in \( \text{sp}^2 \)-hybridized orbitals.
   (c) Place a number symbol (#) on any oxygen atom that is \( \text{sp}^2 \) hybridized as a consequence of having a lone pair in a \( 2p \) orbital.
   (d) Use an arrow to point to any N atom that has trigonal planar geometry.
15. Draw line structures of a molecule with the formula \( \text{C}_5\text{H}_{11}\text{N} \) that has the characteristics outlined in (a), (b), and (c) below.

(a) An \( sp^2 \) nitrogen atom with a conjugated lone pair, one methyl substituent, and one ethyl substituent

(b) A disubstituted trans alkene and a primary amine with an \( sp^3 \) nitrogen connected to an \( sp^3 \) carbon

(c) A three-membered ring containing a secondary \( sp^3 \) nitrogen with cis methyl and ethyl substituents on the ring

ANS:

16. Draw line structures of a molecule with the formula \( \text{C}_4\text{H}_6\text{O} \) that has the characteristics outlined in (a), (b), and (c) below.
(a) Two $sp$-hybridized carbon atoms, a methyl group, and a primary alcohol
(b) An epoxide and one carbon–carbon bond formed from the overlap of $2p$ orbitals
(c) A cyclopropane ring connected to only one substituent via a $\sigma$ bond. This $\sigma$ bond is formed from overlap of one $Csp^3$ and one $Csp^2$ orbital.

ANS:

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>Chemical formula</th>
<th>Chemical formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_4H_6O$</td>
<td>$C_4H_6O$</td>
<td>$C_4H_6O$</td>
</tr>
</tbody>
</table>

DIF: Medium  REF: 3.4 | 3.11
OBJ: Determine the hybridization and geometry for an atom in an organic functional group or molecule.  MSC: Creating