9.1 Molecular Shapes

- Lewis structures give atomic connectivity: they tell us which atoms are physically connected to which atoms.
- The shape of a molecule is determined by its **bond angles**.
  - The angles made by the lines joining the nuclei of the atoms in a molecule are the bond angles.
- Consider **CCl₄**:
  - Experimentally we find all Cl–C–Cl bond angles are 109.5°.
  - Therefore, the molecule cannot be planar.
  - All Cl atoms are located at the vertices of a tetrahedron with the C at its center.
- In order to predict molecular shape, we assume that the valence electrons repel each other.
  - Therefore, the molecule adopts the three-dimensional geometry that minimizes this repulsion.
  - We call this model the **Valence Shell Electron Pair Repulsion (VSEPR)** model.

9.2 The VSEPR Model

- A covalent bond forms between two atoms when a pair of electrons occupies the space between the atoms.
  - This is a **bonding pair** of electrons.
  - Such a region is an **electron domain**.
- A **nonbonding pair** or **lone pair** of electrons defines an electron domain located principally on one atom.
- Example: **NH₃** has three bonding pairs and one lone pair.
- VSEPR predicts that the best arrangement of electron domains is the one that minimizes the repulsions among them.
  - The arrangement of electron domains about the central atom of a molecule is its **electron-domain geometry**.
  - There are five different electron-domain geometries:
    - linear (two electron domains), trigonal planar (three domains), tetrahedral (four domains), trigonal bipyramidal (five domains) and octahedral (six domains).
- The **molecular geometry** is the arrangement of the atoms in space.
  - To determine the shape of a molecule we must distinguish between lone pairs and bonding pairs.
  - We use the electron-domain geometry to help us predict the molecular geometry.
    - Draw the Lewis structure.
    - Count the total number of electron domains around the central atom.
    - Arrange the electron domains in one of the five geometries to minimize electron-electron repulsion.
    - Next, determine the 3-D structure of the molecule.
      - We ignore lone pairs in the molecular geometry.
      - Describe the molecular geometry in terms of the bonded atoms.
      - Multiple bonds are counted as one electron domain.

The Effect of Nonbonding Electrons and Multiple Bonds on Bond Angles

We refine VSEPR to predict and explain slight distortions from “ideal” geometries.
- Consider three molecules with tetrahedral electron domain geometries: **CH₄**, **NH₃**, and **H₂O**.
  - By experiment, the H–X–H bond angle decreases from C (109.5° in CH₄) to N (107° in NH₃) to O (104.5° in H₂O).
  - A bonding pair of electrons is attracted by two nuclei. They do not repel as much as lone pairs which are primarily attracted by only one nucleus.
  - Electron domains for nonbonding electron pairs thus exert greater repulsive forces on adjacent electron domains.
    - They tend to compress the bond angles.
    - The bond angle decreases as the number of nonbonding pairs increases.
  - Similarly, electrons in multiple bonds repel more than electrons in single bonds (e.g., in Cl₂CO the O–C–Cl angle is 124.3°, and the Cl–C–Cl bond angle is 111.4°).
We will encounter eleven basic molecular shapes:

- three atoms (AB$_2$):
  - linear
  - bent
- four atoms (AB$_3$):
  - trigonal planar
  - trigonal pyramidal
  - t-shaped
- five atoms (AB$_4$):
  - tetrahedral
  - square planar
  - seesaw
- six atoms (AB$_5$):
  - trigonal bipyramidal
  - square pyramidal
- seven atoms (AB$_6$):
  - octahedral

<table>
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<td>Trigonal Planar</td>
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<tr>
<td>6</td>
<td>Octahedral</td>
<td>90°</td>
<td>Octahedral</td>
</tr>
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Molecules with Expanded Valence Shells

- Atoms that have expanded octets have five electron domains (trigonal bipyramidal) or six electron domains (octahedral) electron-domain geometries.
  - Trigonal bipyramidal structures have a plane containing three electron pairs.
    - The fourth and fifth electron pairs are located above and below this plane.
    - In this structure two trigonal pyramids share a base.
  - For octahedral structures, there is a plane containing four electron pairs.
    - Similarly, the fifth and sixth electron pairs are located above and below this plane.
    - Two square pyramids share a base.
- Consider a trigonal bipyramid.
  - The three electron pairs in the plane are called equatorial.
  - The two electron pairs above and below this plane are called axial.
  - The axial electron pairs are 180° apart and 90° to the equatorial electrons.
  - The equatorial electron pairs are 120° apart.
  - To minimize electron–electron repulsion, nonbonding pairs are always placed in equatorial positions and bonding pairs are placed in either axial or equatorial positions.
- Consider an octahedron.
  - The four electron pairs in the plane are at 90° to each other.
  - The two axial electron pairs are 180° apart and at 90° to the electrons in the plane.
  - Because of the symmetry of the system, each position is equivalent.
  - If we have five bonding pairs and one lone pair, it does not matter where the lone pair is placed.
    - The molecular geometry is square pyramidal.
  - If two non-bonding pairs are present, the repulsions are minimized by pointing them toward opposite sides of the octahedron.
    - The molecular geometry is square planar.
Shapes of Larger Molecules
• In acetic acid, CH₃COOH, there are three interior atoms: two C and one O.
  • We assign the molecular (and electron-domain) geometry about each interior atom separately:
    • The geometry around the first C is tetrahedral.
    • The geometry around the second C is trigonal planar.
    • The geometry around the O is bent (tetrahedral).

9.3 Molecular Shape and Molecular Polarity
• Polar molecules interact with electric fields.
• We previously saw that binary compounds are polar if their centers of negative and positive charge do not coincide.
  • If two charges, equal in magnitude and opposite in sign, are separated by a distance \( d \), then a dipole is established.
    • The dipole moment, \( \mu \), given by \( \mu = Qr \) where \( Q \) is the magnitude of the charge.
• We can extend this to polyatomic molecules.
  • For each bond in a polyatomic molecule, we can consider the bond dipole.
    • The dipole moment due only to the two atoms in the bond is the bond dipole.
  • Because bond dipoles and dipole moments are vector quantities, the orientation of these individual dipole moments determines whether the molecule has an overall dipole moment.
    • In CO₂ each \(^{\delta^+}\text{C}–\text{O}^{\delta^-}\) dipole is canceled because the molecule is linear.
    • In H₂O, the \(^{\delta^+}\text{H}–\text{O}^{\delta^-}\) dipoles do not cancel because the molecule is bent.
• It is possible for a molecule with polar bonds to be either polar or nonpolar.
• Example:
  • For diatomic molecules:
    • polar bonds always result in an overall dipole moment.
  • For triatomic molecules:
    • if the molecular geometry is bent, there is an overall dipole moment.
    • if the molecular geometry is linear and the B atoms are the same, there is no overall dipole moment.
    • if the molecular geometry is linear and the B atoms are different, there is an overall dipole moment.
  • For molecules with four atoms:
    • if the molecular geometry is trigonal pyramidal, there is an overall dipole moment.
    • if the molecular geometry is trigonal planar and the B atoms are identical, there is no overall dipole \( \mu \).
    • if the molecular geometry is trigonal planar and the B atoms are different, there is an overall dipole \( \mu \).

9.4 Covalent Bonding and Orbital Overlap
• Lewis structures and VSEPR theory give us the shape and location of electrons in a molecule.
• They do not explain why a chemical bond forms.
• How can quantum mechanics be used to account for molecular shape? What orbitals are involved in bonding?
• We use valence-bond theory.
  • A covalent bond forms when the orbitals on two atoms overlap.
    • The shared region of space between the orbitals is called the orbital overlap.
    • There are two electrons (usually one from each atom) of opposite spin in the orbital overlap.
  • As two nuclei approach each other their atomic orbitals overlap.
  • As the amount of overlap increases, the energy of the interaction decreases.
  • At some distance the minimum energy is reached.
    • The minimum energy corresponds to the bonding distance (or bond length).
  • As the two atoms get closer, their nuclei begin to repel and the energy increases.
  • At the bonding distance, the attractive forces between nuclei and electrons just balance the repulsive forces (nucleus-nucleus, electron-electron).

9.5 Hybrid Orbitals
• We can apply the idea of orbital overlap and valence-bond theory to polyatomic molecules.

\textit{sp} Hybrid Orbitals
• Consider the BeF₂ molecule.
  • Be has a 1s²2s² electron configuration.
  • There is no unpaired electron available for bonding.
  • We conclude that the atomic orbitals are not adequate to describe orbitals in molecules.
• We know that the F–Be–F bond angle is 180° (VSEPR theory).
• We also know that one electron from Be is shared with each one of the unpaired electrons from F.
• We assume that the Be orbitals in the Be–F bond are 180° apart.
• We could promote an electron from the 2s orbital on Be to the 2p orbital to get two unpaired electrons for bonding.
  • BUT the geometry is still not explained.
• We can solve the problem by allowing the 2s and one 2p orbital on Be to mix or form two new hybrid orbitals (a process called hybridization).
  • The two equivalent hybrid orbitals that result from mixing an s and a p orbital and are called sp hybrid orbitals.
  • The two lobes of an sp hybrid orbital are 180° apart.
  • According to the valence-bond model, a linear arrangement of electron domains implies sp hybridization.
  • Since only one of 2p orbitals of Be has been used in hybridization, there are two unhybridized p orbitals remaining on Be.
  • The electrons in the sp hybrid orbital form shared electron bonds with the two fluorine atoms.

**sp² and sp³ Hybrid Orbitals**

• Important: when we mix n atomic orbitals we must get n hybrid orbitals.
• Three sp² hybrid orbitals are formed from hybridization of one s and two p orbitals.
  • Thus, there is one unhybridized p orbital remaining.
  • The large lobes of the sp² hybrids lie in a trigonal plane.
  • Molecules with trigonal planar electron-pair geometries have sp² orbitals on the central atom.
• Four sp³ hybrid orbitals are formed from hybridization of one s and three p orbitals.
  • Therefore, there are four large lobes.
  • Each lobe points towards the vertex of a tetrahedron.
  • The angle between the large lobes is 109.5°.
  • Molecules with tetrahedral electron pair geometries are sp³ hybridized.

**Hybridization Involving d Orbitals**

• Since there are only three p orbitals, trigonal bipyramidal and octahedral electron-pair geometries must involve d orbitals.
• Trigonal bipyramidal electron pair geometries require sp³d hybridization.
• Octahedral electron pair geometries require sp³d² hybridization.
• Electron pair VSEPR geometry corresponds well with the hybridization.
  • Use of d orbitals in making hybrid orbitals corresponds well with the idea of an expanded octet.

**Summary** - We need to know the electron-domain geometry before we can assign hybridization.
• To assign hybridization:
  • Draw a Lewis structure.
  • Assign the electron-domain geometry using VSEPR theory.
  • Specify the hybridization required to accommodate the electron pairs based on their geometric arrangement.
  • Name the geometry by the positions of the atoms.

**9.6 Multiple Bonds** - In the covalent bonds we have seen so far the electron density has been concentrated symmetrically about the internuclear axis.

• **Sigma (σ) bonds**: electron density lies on the axis between the nuclei.
  • All single bonds are σ bonds.
• What about overlap in multiple bonds?
  • **Pi (π) bonds**: electron density lies above and below the plane of the nuclei.
  • A double bond consists of one σ bond and one π bond.

**Bond Order**

• A triple bond has one σ bond and two π bonds.
• Bond order = 1 for a single bond.
• Bond order = 2 for a double bond.
• Bond order = 3 for a triple bond.

• Often, the p orbitals involved in π bonding come from unhybridized orbitals.
• For example: ethylene, C₂H₄, has:
  • One σ and one π bond.
  • Both C atoms are sp² hybridized.
  • Both C atoms have trigonal planar electron-pair and molecular geometries.
• For example: acetylene, C₂H₂:
  • The electron-domain geometry of each C is linear.
  • Therefore, the C atoms are sp hybridized.
  • The sp hybrid orbitals form the C–C and C–H σ bonds.
  • There are two unhybridized p orbitals on each C atom.
Both unhybridized $p$ orbitals form the two $\pi$ bonds;
   - One $\pi$ bond is above and below the plane of the nuclei;
   - One $\pi$ bond is in front and behind the plane of the nuclei.

For triple bonds, one $\pi$ bond is always above and below and the other is in front and behind the plane of the nuclei.

**Delocalized $\pi$ Bonding** - So far all the bonds we have encountered are localized between two nuclei.

- In the case of benzene:
  - There are six C–C $\sigma$ bonds and six C–H $\sigma$ bonds.
  - Each C atom is $sp^2$ hybridized.
  - There is one unhybridized $p$ orbital on each carbon atom, resulting in six unhybridized carbon $p$ orbitals in a ring.

- In benzene there are two options for the three $\pi$ bonds:
  - localized between carbon atoms or
  - delocalized over the entire ring (i.e., the $\pi$ electrons are shared by all six carbon atoms).

- Experimentally, all C–C bonds are the same length in benzene. Therefore, all C–C bonds are of the same type (recall single bonds are longer than double bonds).

**General Conclusions**

- Every pair of bonded atoms shares one or more pairs of electrons.
- Two electrons shared between atoms on the same axis as the nuclei are $\sigma$ bonds.
- $\sigma$ bonds are always localized in the region between two bonded atoms.
- If two atoms share more than one pair of electrons, the additional pairs form $\pi$ bonds.
- When resonance structures are possible, delocalization is also possible.

**9.7 Molecular Orbitals** WE ARE NOT GOING TO LEARN THIS MO STUFF!!

- Some aspects of bonding are not explained by Lewis structures, VSEPR theory, and hybridization.

- For these molecules, we use molecular orbital (MO) theory.
- Just as electrons in atoms are found in atomic orbitals, electrons in molecules are found in molecular orbitals.
  - However, unlike atomic orbitals, molecular orbitals are associated with an entire molecule.

**Homework Problems**

Pg 388 #4, #13, #17, #19, #21, #25, #31, #33, #35, #75, #82  
Pg 388 #8, #40, #43, #44, #47, #49, #51, #53, #56, #65A
1) For a molecule with the formula $\text{AB}_2$, the molecular shape is __________.
A) linear or bent  B) linear or trigonal planar  C) linear or T-shaped  D) T-shaped  E) trigonal planar

2) According to VSEPR theory, if there are four electron domains in the valence shell of an atom, they will be arranged in a(n) __________ geometry.
A) octahedral  B) linear  C) tetrahedral  D) trigonal planar  E) trigonal bipyramidal

3) The electron-domain geometry and molecular geometry of iodine trichloride are __________ and __________, respectively.
A) trigonal bipyramidal, trigonal planar  B) tetrahedral, trigonal pyramidal  C) trigonal bipyramidal, T-shaped  D) octahedral, trigonal planar  E) T-shaped, trigonal planar

4) The molecular geometry of ________ is square planar.
A) ________ B) ________ C) ________ D) ________ E) ________

5) The molecular geometry of the $\text{H}_3\text{O}^+$ ion is ________.
A) linear  B) tetrahedral  C) bent  D) octahedral  E) octahedral

6) The F–B–F bond angle in the BF$_3$ molecule is ________.
A) 90°  B) 109.5°  C) 120°  D) 180°  E) 60°

7) The O–S–O bond angle in SO$_2$ is slightly less than ________.
A) 90°  B) 109.5°  C) 120°  D) 180°  E) 60°

8) According to valence bond theory, which orbitals on bromine atoms overlap in the formation of the bond in Br$_2$?
A) 3s  B) 3p  C) 4s  D) 4p  E) 3d

9) The electron-domain geometry of a sulfur-centered compound is trigonal bipyramidal. The hybridization of the central sulfur atom is ________.
A) $sp$  B) $sp^2$  C) $sp^3$  D) $sp^3d$  E) $sp^3d^2$

10) The hybridization of orbitals on the central atom in a molecule is sp. The electron-domain geometry around this central atom is ________.
A) octahedral  B) linear  C) trigonal planar  D) trigonal bipyramidal  E) tetrahedral

11) In order to produce $sp^3$ hybrid orbitals, ________ s atomic orbital(s) and ________ p atomic orbital(s) must be mixed.
A) one, two  B) one, three  C) one, one  D) two, two  E) two, three

12) The angles between $sp^3$ orbitals are ________.
A) 45°  B) 109.5°  C) 90°  D) 120°  E) 180°

13) There are ________ σ and ________ π bonds in the $\text{H}–\text{C}≡\text{C}–\text{H}$ molecule.
A) 3 and 2  B) 3 and 4  C) 4 and 3  D) 2 and 3  E) 5 and 0

14) The total number of π bonds in the $\text{H}–\text{C}≡\text{C}–\text{C}≡\text{N}$ molecule is ________.
A) 3  B) 4  C) 6  D) 9  E) 12

15) There is/are ________ σ bond(s) in the molecule below.
A) 1  B) 2  C) 12  D) 13  E) 18

16) The basis of the VSEPR model of molecular bonding is ________.
A) regions of electron density on an atom will organize themselves so as to maximize $s$-character  B) regions of electron density in the valence shell of an atom will arrange themselves so as to maximize overlap  C) atomic orbitals of the bonding atoms must overlap for a bond to form  D) electron domains in the valence shell of an atom will arrange themselves so as to minimize repulsions  E) hybrid orbitals will form as necessary to, as closely as possible, achieve spherical symmetry

17) The O–C–O bond angle in the CO$_3^{2-}$ ion is approximately ________.
A) 90°  B) 109.5°  C) 120°  D) 180°  E) 60°

18) The Cl–C–Cl bond angle in the CC$I_2$O molecule (C is the central atom) is slightly ________.
A) greater than 90°  B) less than 109.5°  C) less than 120°  D) greater than 120°  E) greater than 109.5°
19) The bond angles marked a, b, and c in the molecule below are about __________, __________, and __________, respectively.

   ![Molecule Image]

A) 90°, 90°, 90°  B) 120°, 120°, 90°  C) 120°, 120°, 109.5°  D) 109.5°, 120°, 109.5°  E) 109.5°, 90°, 120°

20) The central iodine atom in the \( \text{ICl}_4^- \) ion has __________ nonbonded electron pairs and __________ bonded electron pairs in its valence shell.

   A) 2, 2  B) 3, 4  C) 1, 3  D) 3, 2  E) 2, 4

21) The central Xe atom in the XeF\(_4\) molecule has __________ unbonded electron pairs and __________ bonded electron pairs in its valence shell.

   A) 1, 4  B) 2, 4  C) 4, 0  D) 4, 1  E) 4, 2

22) An electron domain consists of __________.

   a) a nonbonding pair of electrons  
   b) a single bond  
   c) a multiple bond

   A) a only  B) b only  C) c only  D) a, b, and c  E) b and c

23) According to VSEPR theory, if there are three electron domains on a central atom, they will be arranged such that the angles between the domains are __________.

   A) 90°  B) 180°  C) 109.5°  D) 360°  E) 120°

24) The electron-domain geometry and the molecular geometry of a molecule of the general formula \( \text{AB}_n \) are __________.

   A) never the same  B) always the same  C) sometimes the same  D) not related  E) mirror images of one another

25) For molecules of the general formula \( \text{AB}_n \), \( n \) can be greater than four __________.

   A) for any element A  B) only when A is an element from the third period or below the third period  
   C) only when A is boron or beryllium  D) only when A is carbon  E) only when A is Xe

26) Of the molecules below, only __________ is polar.

   A) \( \text{Sbf}_5 \)  B) \( \text{AsH}_3 \)  C) \( \text{I}_2 \)  D) \( \text{SF}_6 \)  E) \( \text{CH}_4 \)

27) Of the molecules below, only __________ is nonpolar.

   A) \( \text{BF}_3 \)  B) \( \text{NF}_3 \)  C) \( \text{IF}_3 \)  D) \( \text{PBr}_3 \)  E) \( \text{BrCl}_3 \)

28) Three monosulfur fluorides are observed: \( \text{SF}_2 \), \( \text{SF}_4 \), and \( \text{SF}_6 \). Of these, __________ is/are polar.

   A) \( \text{SF}_2 \) only  B) \( \text{SF}_4 \) and \( \text{SF}_4 \) only  C) \( \text{SF}_4 \) only  D) \( \text{SF}_6 \) only  E) \( \text{SF}_2 \), \( \text{SF}_4 \), and \( \text{SF}_6 \)

29) The molecular geometry of the \( \text{BeCl}_4 \) molecule is __________, and this molecule is __________.

   A) linear, nonpolar  B) linear, polar  C) bent, nonpolar  D) bent, polar  E) trigonal planar, polar

30) Of the following molecules, only __________ is polar.

   A) \( \text{BeCl}_2 \)  B) \( \text{BF}_3 \)  C) \( \text{CBr}_4 \)  D) \( \text{SiH}_2\text{Cl}_2 \)  E) \( \text{Cl}_2 \)

31) Of the following, only _____ has \( sp^2 \) hybridization of the central atom.

   A) \( \text{PH}_3 \)  B) \( \text{CO}_3^{2-} \)  C) \( \text{ICl}_3 \)  D) \( \text{I}_3^- \)  E) \( \text{PF}_5 \)

32) The \( sp^3d^2 \) atomic hybrid orbital set accommodates __________ electron domains.

   A) 2  B) 3  C) 4  D) 5  E) 6

33) The hybridizations of iodine in \( \text{IF}_3 \) and \( \text{IF}_5 \) are __________ and __________, respectively.

   A) \( sp^3 \), \( sp^3d \)  B) \( sp^3d \), \( sp^3d^2 \)  
   C) \( sp^3d \), \( sp^3 \)  D) \( sp^3d^2 \), \( sp^3d \)  
   E) \( sp^3d^2 \), \( sp^3d^2 \)

34) __________ hybrid orbitals are used for bonding by Xe in the \( \text{XeF}_4 \) molecule.

   A) \( sp^2 \)  B) \( sp^3 \)  C) \( sp^3d \)  D) \( sp^3d^2 \)  E) \( sp \)
Consider the following species when answering the following questions:
(i) \( \text{PCl}_3 \) (ii) \( \text{CCl}_4 \) (iii) \( \text{TeCl}_4 \) (iv) \( \text{XeF}_4 \)
(v) \( \text{SF}_6 \)

35) In which of the molecules does the central atom utilize d orbitals to form hybrid orbitals?
A) (i) and (ii)  
B) (iii) only  
C) (i) and (v)  
D) (iii), (iv), and (v)  
E) (v) only

36) Which of the molecules has a see-saw shape?
A) (i)  
B) (ii)  
C) (iii)  
D) (iv)  
E) (v)

37) In which of the molecules is the central atom \( \text{sp}^3\text{d}^2 \) hybridized?
A) (i) and (ii)  
B) (iii) only  
C) (iii) and (iv)  
D) (iv) and (v)  
E) (v) only

38) The blending of one s atomic orbital and two p atomic orbitals produces __________.
A) three \( \text{sp} \) hybrid orbitals  
B) two \( \text{sp}^3 \) hybrid orbitals  
C) three \( \text{sp}^3 \) hybrid orbitals  
D) two \( \text{sp}^3 \) hybrid orbitals  
E) three \( \text{sp}^2 \) hybrid orbitals

39) A typical double bond __________.
A) is stronger and shorter than a single bond  
B) consists of one \( \sigma \) bond and one \( \pi \) bond  
C) imparts rigidity to a molecule  
D) consists of two shared electron pairs  
E) All of the above answers are correct.

40) In a polyatomic molecule, "localized" bonding electrons are associated with __________.
A) one particular atom  
B) two particular atoms  
C) all of the atoms in the molecule  
D) all of the \( \sigma \) bonds in the molecule  
E) two or more \( \sigma \) bonds in the molecule

41) Which of the following molecules or ions will exhibit delocalized bonding?
\( \text{SO}_2 \quad \text{SO}_3 \quad \text{SO}_3^{2-} \)
A) \( \text{SO}_2, \text{SO}_3, \text{and} \ \text{SO}_3^{2-} \)  
B) \( \text{SO}_3^{2-} \) only  
C) \( \text{SO}_2 \) and \( \text{SO}_3 \)  
D) \( \text{SO}_3 \) and \( \text{SO}_3^{2-} \)  
E) None of the above will exhibit delocalized bonding.

42) In order to exhibit delocalized \( \pi \) bonding, a molecule must have __________.
A) at least two \( \pi \) bonds  
B) at least two resonance structures  
C) at least three \( \sigma \) bonds  
D) at least four atoms  
E) trigonal planar electron domain geometry

43) The carbon-carbon \( \sigma \) bond in ethylene, \( \text{CH}_2\text{CH}_2 \), results from the overlap of __________.
A) \( \text{sp} \) hybrid orbitals  
B) \( \text{sp}^3 \) hybrid orbitals  
C) \( \text{sp}^2 \) hybrid orbitals  
D) \( s \) atomic orbitals  
E) \( p \) atomic orbitals

44) The \( \pi \) bond in ethylene, \( \text{CH}_2\text{CH}_2 \), results from the overlap of __________.
A) \( \text{sp}^3 \) hybrid orbitals  
B) \( s \) atomic orbitals  
C) \( \text{sp} \) hybrid orbitals  
D) \( \text{sp}^2 \) hybrid orbitals  
E) \( p \) atomic orbitals

45) In order for rotation to occur about a double bond, __________.
A) the \( \sigma \) bond must be broken  
B) the \( \pi \) bond must be broken  
C) the bonding must be delocalized  
D) the bonding must be localized  
E) the \( \sigma \) and \( \pi \) bonds must both be broken

46) The \( \text{N–N} \) bond in \( \text{HNNH} \) consists of __________.
A) one \( \sigma \) bond and one \( \pi \) bond  
B) one \( \sigma \) bond and two \( \pi \) bonds  
C) two \( \sigma \) bonds and one \( \pi \) bond  
D) two \( \sigma \) bonds and two \( \pi \) bonds  
E) one \( \sigma \) bond and no \( \pi \) bonds

47) Electrons in __________ bonds remain localized between two atoms. Electrons in __________ bonds can become delocalized between more than two atoms.
A) \( \pi \) and \( \sigma \)  
B) \( \sigma \) and \( \pi \)  
C) \( \sigma \) and \( \sigma \)  
D) \( \sigma \) and \( \pi \)  
E) ionic, \( \sigma \)