



# ScienceGuyz

## CHEM 2211

### Chapter 1:

# Atomic Structure and Hybridization

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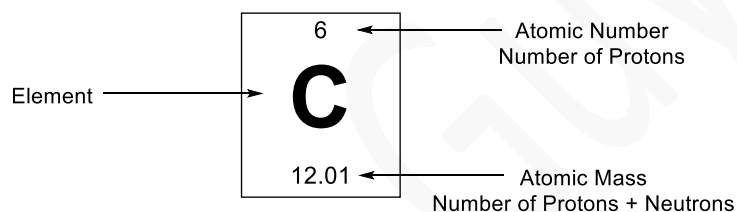
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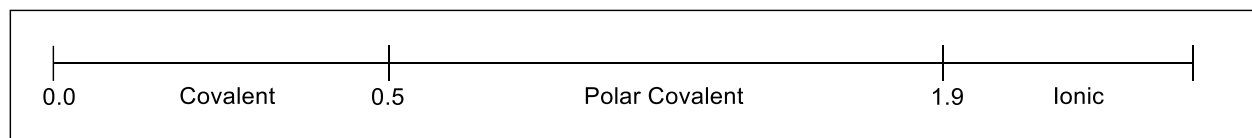
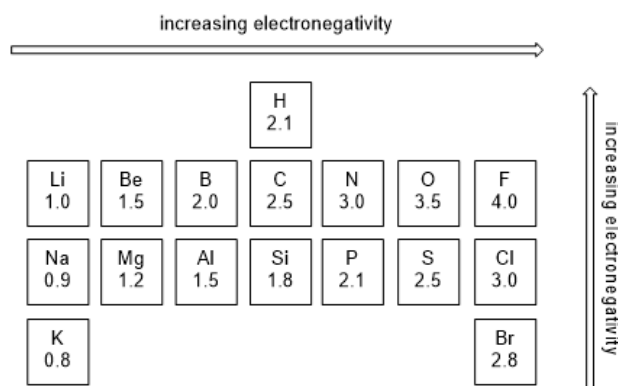
### Introduction to Organic Chemistry:

- I. **Inorganic compounds** are derived from non-living sources.
- II. **Organic compounds** are derived from living organisms, such as plants and animals.
- III. **Composition of Atoms:** atoms are composed of protons, neutrons, and electrons.
  - a. **Protons:** Positively charged particles found in the nucleus of an atom. The number of protons in an atom corresponds to the **atomic number** of the atom, which identifies an atom as a particular type of element.
  - b. **Neutrons:** Neutral (no charge) particles found in the nucleus of an atom. Neutrons add to the atomic mass of an atom. Different *isotopes* of an element vary in number of neutrons.
  - c. **Electrons:** Negatively charged species that orbit the nucleus of an atom. The mass of electrons is extremely small relative to that of neutrons and protons. The number of electrons and protons in an atom will always be equal for neutral atoms.



IV. **Electronegativity** is the tendency of an atom to attract electron density towards itself, causing unequal electron distribution in bonds. Chemists classify bond types based on the extent of sharing, which can be calculated using electronegativity values.

- a. **Ionic bonds** form when the electronegativity difference exceeds 1.9, leading to an attraction between oppositely charged ions rather than shared electrons.
- b. **Covalent bonds** form when the electronegativity difference is less than 0.5, resulting in equal electron sharing.
- c. **Polar covalent bonds** form from an electronegativity difference between 0.5 and 1.9, where one atom pulls electrons more strongly, causing induction.



**Example:** Classify the following bonds as being either covalent, polar covalent, or ionic. If the bond is polar covalent, indicate the direction of the dipole.

C-H	C-Na	O-K	O-O	F-C
<input type="checkbox"/> Covalent	<input type="checkbox"/> Covalent	<input type="checkbox"/> Covalent	<input type="checkbox"/> Covalent	<input type="checkbox"/> Covalent
<input type="checkbox"/> Polar Covalent	<input type="checkbox"/> Polar Covalent	<input type="checkbox"/> Polar Covalent	<input type="checkbox"/> Polar Covalent	<input type="checkbox"/> Polar Covalent
<input type="checkbox"/> Ionic	<input type="checkbox"/> Ionic	<input type="checkbox"/> Ionic	<input type="checkbox"/> Ionic	<input type="checkbox"/> Ionic

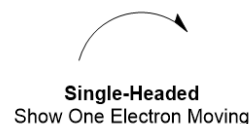
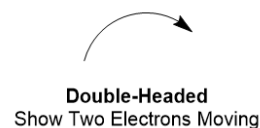
- V. In this course, we will explore the process of covalent bond breakage, which can occur through either homolytic or heterolytic cleavage.
- Homolytic cleavage** breaks a non-polar covalent bond, with each atom retaining one electron, forming radicals.
  - Heterolytic cleavage** breaks a polar covalent bond, with the more electronegative atom retaining both electrons, forming an anion.

**Example:** Predict whether the indicated bond will cleave homolytically or heterolytically.

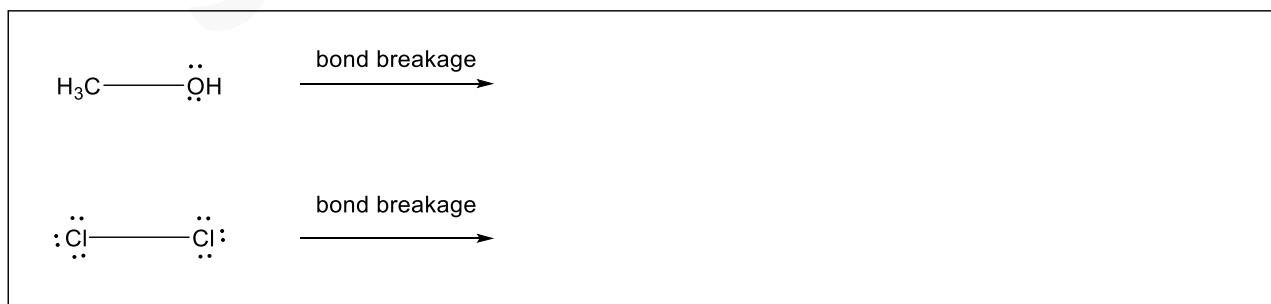
H <sub>3</sub> C—OH	Cl—Cl	H <sub>3</sub> C—H	H <sub>2</sub> N—H
<input type="checkbox"/> Homolytically	<input type="checkbox"/> Homolytically	<input type="checkbox"/> Homolytically	<input type="checkbox"/> Homolytically
<input type="checkbox"/> Heterolytically	<input type="checkbox"/> Heterolytically	<input type="checkbox"/> Heterolytically	<input type="checkbox"/> Heterolytically

VI. **Curvy arrows** are used to depict electron movement, where a double-headed arrow shows an electron pair moving and a single-headed arrow (fishhook) shows a single electron moving. The arrow shows the direction of electron flow: from the source to the destination.

- Curved arrows that start from a bond indicate the breakage of the bond, with the electron movement dependent on the type of bond (polar vs non-polar).



**Example:** Demonstrate how the bonds below will cleave using curvy arrows. Additionally, show the products of the bonds breaking.



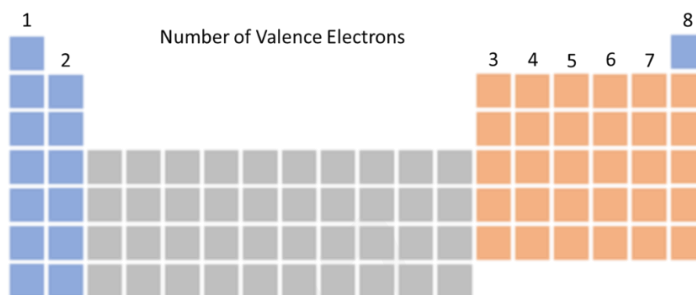
### Lewis & Kekulé Structures:

I. **Lewis structures** are structural representations of a molecule/atom/ion that show all valence electrons and charges.

- a. Preferred bonding arrangements allow us to predict how atoms are likely to behave in molecules, minimizing charge imbalances. These arrangements are determined by the number of valence electrons each atom possesses.

1. Carbon: 4 bonds, no lone pairs
2. Nitrogen: 3 bonds, 1 lone pair
3. Oxygen: 2 bonds, 2 lone pairs
4. Halogens: 1 bond, 3 lone pairs

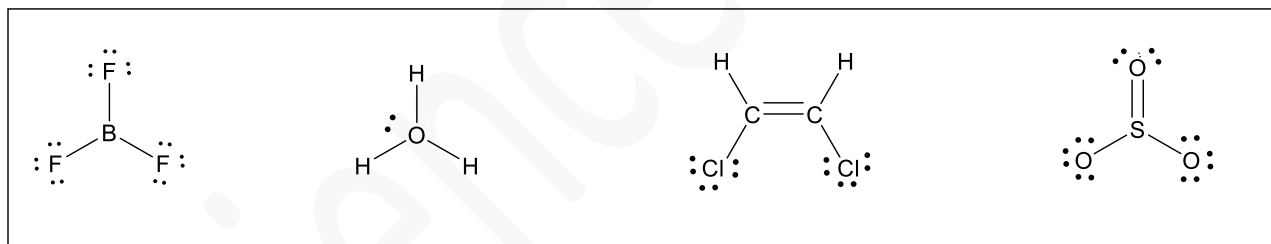
- b. Formal charges occur when an atom deviates from its expected number of valence electrons. Use the equation below to calculate the formal charge of an atom.



$$\text{Formal Charge} = (\# \text{ valence electrons}) - (\# \text{ of nonbonding electrons}) - 1/2(\# \text{ of bonding electrons})$$

$$\text{Formal Charge} = (\# \text{ valence electrons}) - (\# \text{ of dots}) - (\# \text{ of lines})$$

**Example:** Determine the missing formal charges, if any, on the molecules shown below.



- c. To assemble a Lewis structure, follow these steps:

1. **Sum the total number of valence electrons.** For neutral molecules, this is simply the sum of the valence electrons of each atom. For ions, adjust the count by adding electrons for negative charges or subtracting electrons for positive charges.
2. **Determine the central atom(s) of the compound.** This is typically the most electropositive atom, or the atom that can make the greatest number of bonds. In organic molecules, the central atom will always be carbon.
3. **Add valence electrons to the central atom.** Add the number of valence electrons which the central atom has been designated to have to the central atom.
4. **Connect atoms via covalent bonds.** Make bonds connecting the central atom to other atoms such that each atom gains an octet.
5. **Insert multiple bonds.** Double or triple bonds sometimes may be made to satisfy the octet rule. Insert these one at a time, as needed.

6. **Assign formal charges.** Assign formal charge to each atom in the structure that has a formal charge different than zero.
- Some formulas may yield multiple valid structures. The most favored structure will be the one that minimizes formal charges overall.

**II. Exceptions to the Octet Rule:** while most atoms prefer to have a full octet, there are a few exceptions that we will encounter in this course.

- Atoms which have fewer than eight valence electrons:
  - Hydrogen only needs two electrons to obtain a full outer shell, and the element can also be stable with zero electrons.
  - Boron and beryllium can be stable with fewer than 8 electrons: six in the case of boron, and four in the case of beryllium.
- Atoms which have more than eight valence electrons:
  - Non-metals in period 3 or higher can exceed the octet rule and maintain more than 8 electrons around their nuclei (ex. Cl, Br, S, P, Ar, Kr, Sn, Sb, Xe) due to the d-orbital.

**Example:** Propose a valid Lewis structure for the formulas listed below.

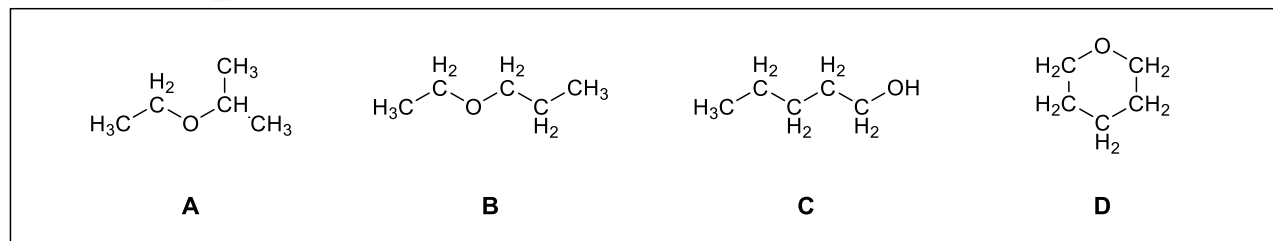
$\text{BF}_4^-$	$\text{HNO}_3$	$\text{CH}_2\text{O}$	$\text{C}_2\text{H}_6$

**III. Kekulé structures**, another structural representation, are drawn like Lewis structures but omit the lone pairs.

**IV.** Lewis structures have their limitations in organic chemistry as we primarily deal with compounds involving several atoms of the same type, allowing for several different valid structures.

- Constitutional Isomers:** compounds that have the same molecular formula but differ in their connectivity. These compounds will have different physical properties.

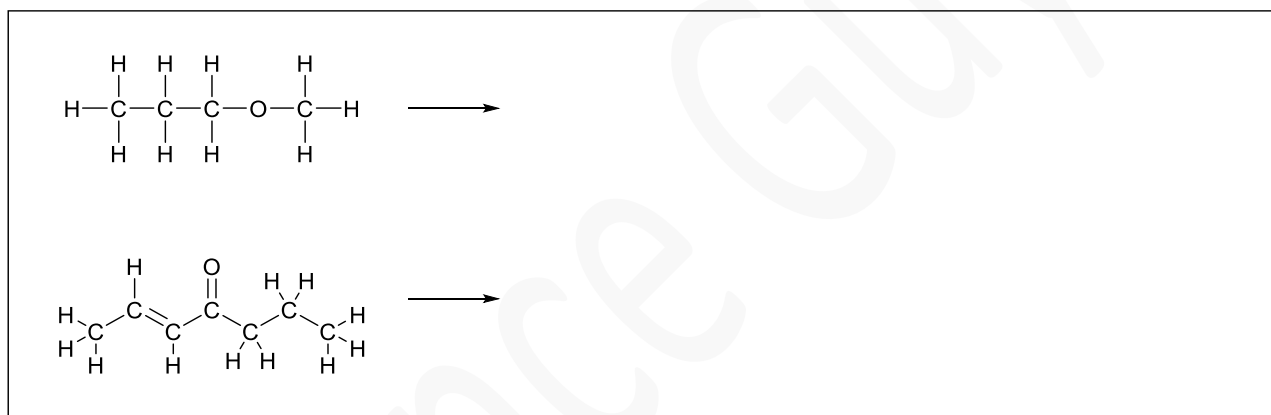
**Example:** Which of these is NOT a constitutional isomer of the other three?



### Other Structural Representations: Condensed and Skeletal

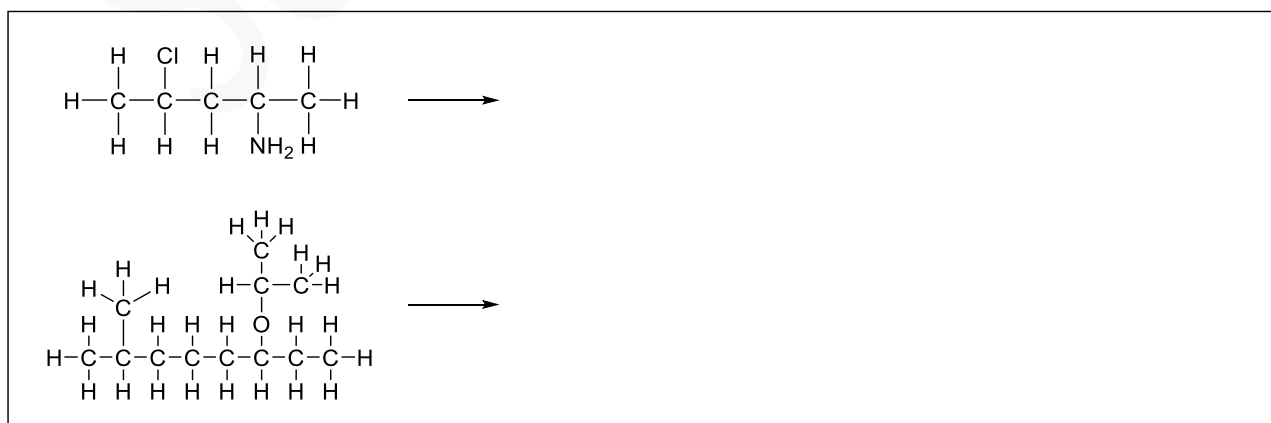
- I. **Condensed formulas** represent an organic compound by omitting some or all covalent bonds, with atoms attached to a particular carbon listed directly after it, using subscripts for multiple identical groups (ex.  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$ ).
  - a. By convention, condensed formulas are read and written from left to right. Starting with the carbon furthest left in the chain, identify each carbon and the number of hydrogen atoms attached to it as you move to the right.
  - b. If multiple hydrogen atoms are attached to any one carbon, only draw one hydrogen atom and designate the number of hydrogen atoms that are attached to the carbon with a subscript (ex.  $\text{CH}_4$ ).
  - c. Heteroatoms (non-carbon or hydrogen atoms) which are attached to a carbon should be written after the hydrogen atoms attached to the carbon (ex.  $\text{CH}_3\text{Br}$ , not  $\text{CBrH}_3$ ).

**Example:** Convert the following Kekulé structures into condensed structure.



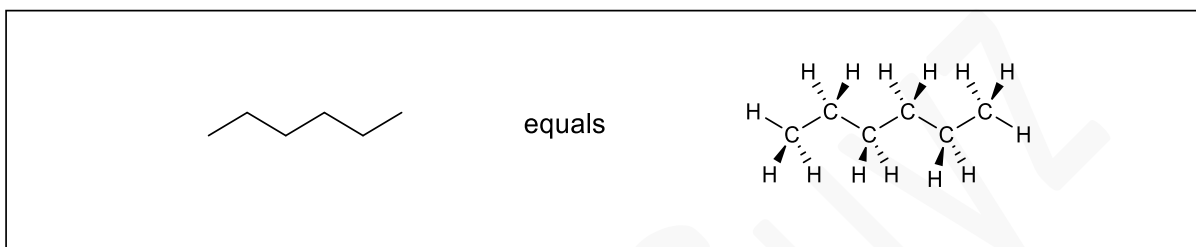
- i. When there are groups of atoms (more than one atom) coming off your continuous chain, these are known as **substituents**. Substituents will always be placed in parenthesis and listed after hydrogen atoms.
  1. Sometimes you will have branching within substituents and in these cases, you will have to use multiple sets of parentheses.

**Example:** Convert the following Kekulé structures into condensed formulas.

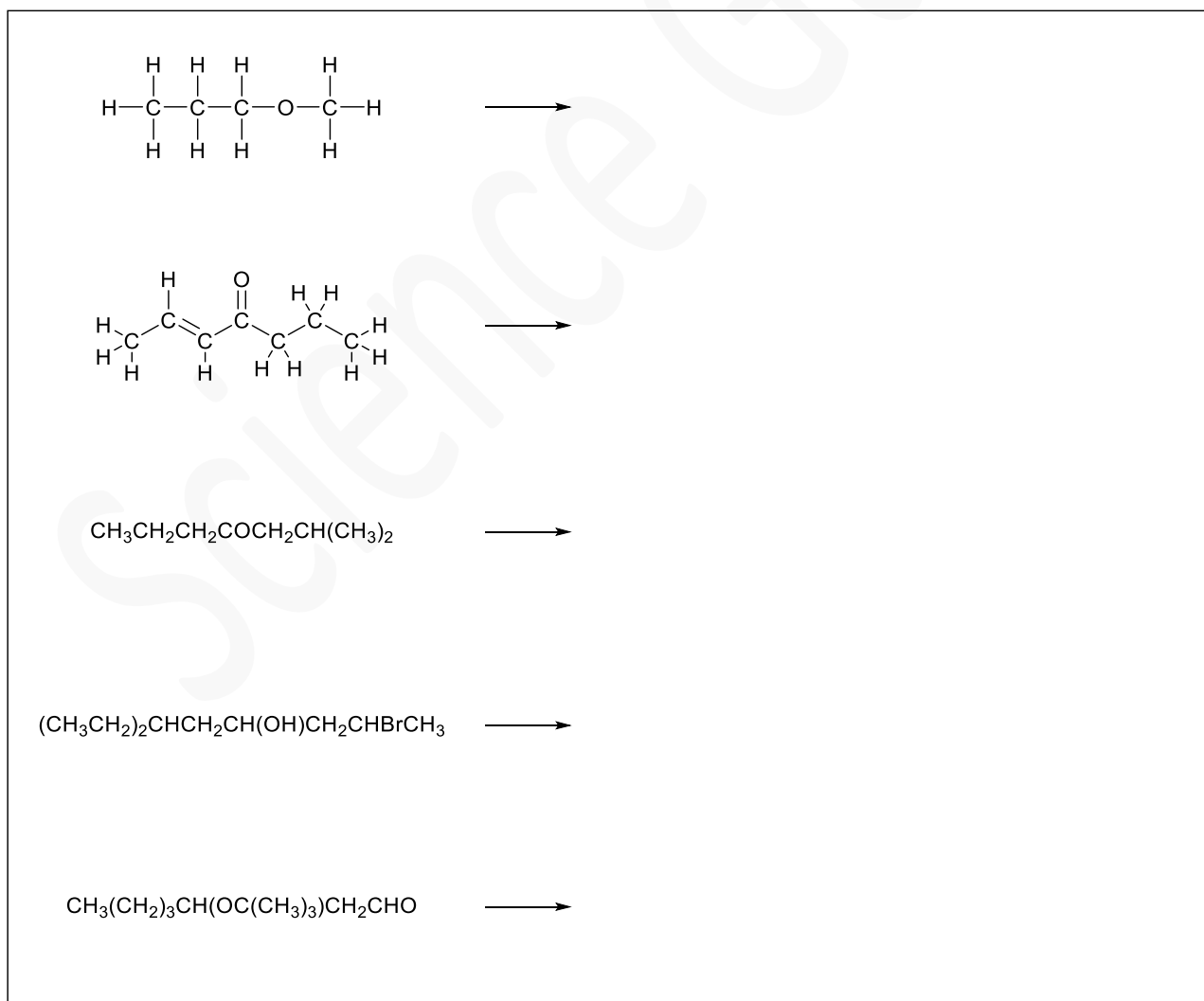


**II. Skeletal Structures (Bond-Line Structures):** A method of depicting carbon and hydrogen atoms in a molecule in a quick and concise manner using zig-zag lines. This is the form that you will see most often throughout this course.

- Each vertex represents a carbon, and it is assumed that hydrogen atoms fill the valence of carbon. Neutral carbon atoms must make four bonds to satisfy the octet rule. Carbanions, carbocations, and carbon radicals make 3 bonds.
- Any atom besides carbon must be drawn out, in addition to any hydrogen atoms attached thereto.



**Example:** Convert the following Kekulé and condensed structures into skeletal structures.

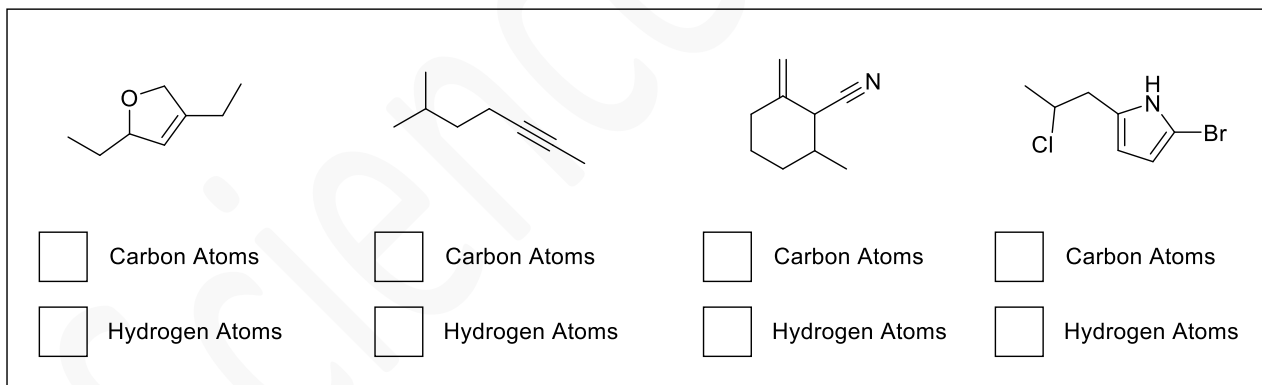




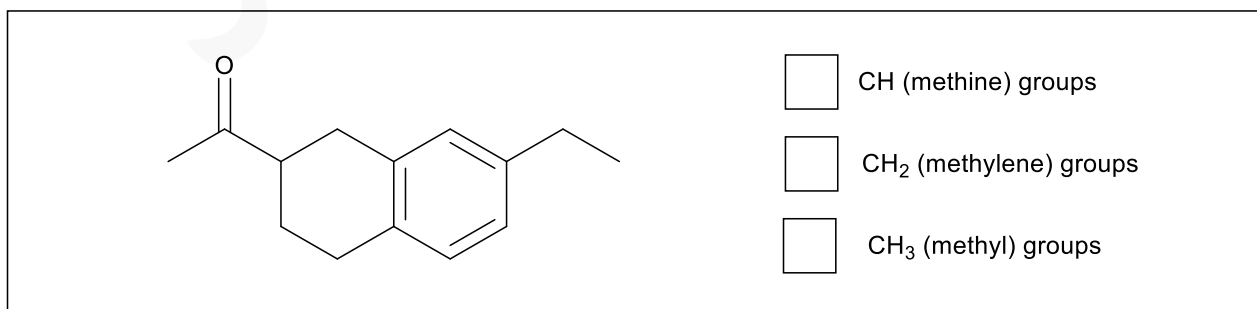
**Example:** Convert the following skeletal structure into condensed structures.



**Example:** How many carbons and hydrogens are present on the compounds shown below?

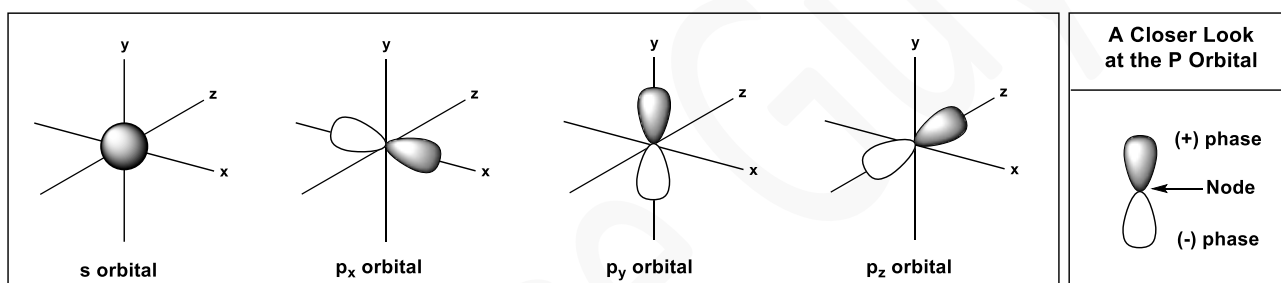


**Example:** How many CH, CH<sub>2</sub>, and CH<sub>3</sub> groups are present on the compound below?



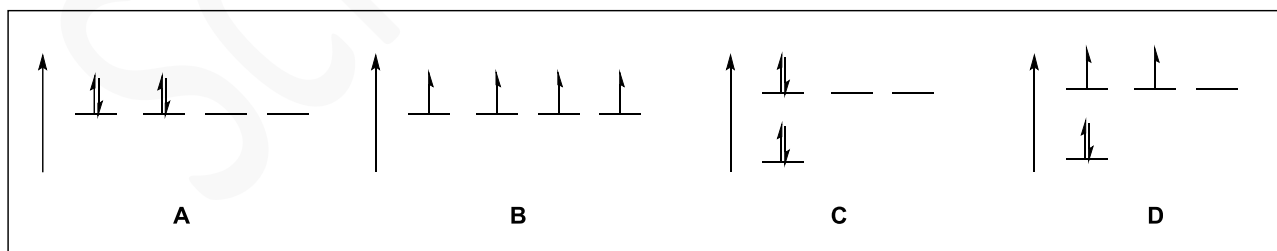
### The Theory of Bonding:

- I. Atoms must bond with each other to create molecules, and that bonding involves the interaction of electrons. Recall from general chemistry that electrons are organized according to their energy level ( $n = 1, n = 2$ , etc.) and sub-level (s, p, d, f) known as **atomic orbitals**. In organic chemistry, we are primarily concerned with the s and p orbitals.
- II. **Atomic orbitals** are a region of space surrounding the nucleus of an atom where an electron is likely to be found; this is also referred to as the electron cloud. The shape of this cloud depends on the nucleus of the atom. The different shapes/types of particular focus in this course are shown below.
  - a. Electrons found in the s-orbital are the lowest in energy as they are closest to the nucleus.
  - b. The three p-orbitals are referred to as **degenerate** orbitals, meaning they all have the same energy level and are higher in energy than the s-orbital. These orbitals also exhibit different phases, which are represented by their shading. The boundary between the shaded regions is known as a **node**.



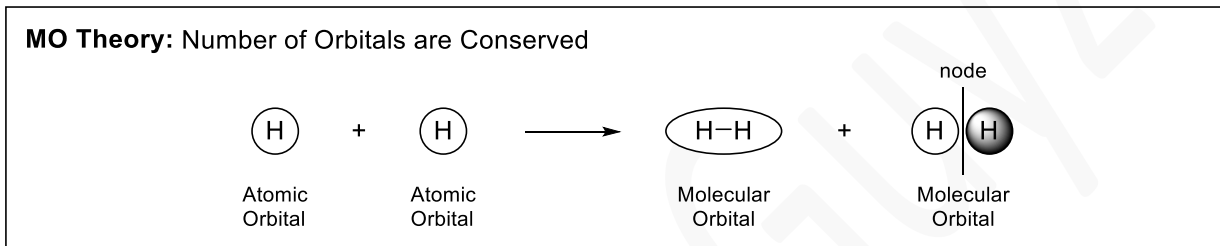
- III. Recall that each orbital can hold two electrons, and electron filling must follow the principles below:
  - a. **The Aufbau principle:** lower energy orbitals are filled first.
  - b. **The Pauli Exclusion principle:** each orbital can accommodate two electrons; those electrons must have opposite spins.
  - c. **Hund's rule:** Degenerate orbitals must be filled individually before spin-pairing.

**Example:** Which diagram correctly depicts the atomic orbital diagram for the valence electrons of a carbon atom in its ground state, prior to hybridization?

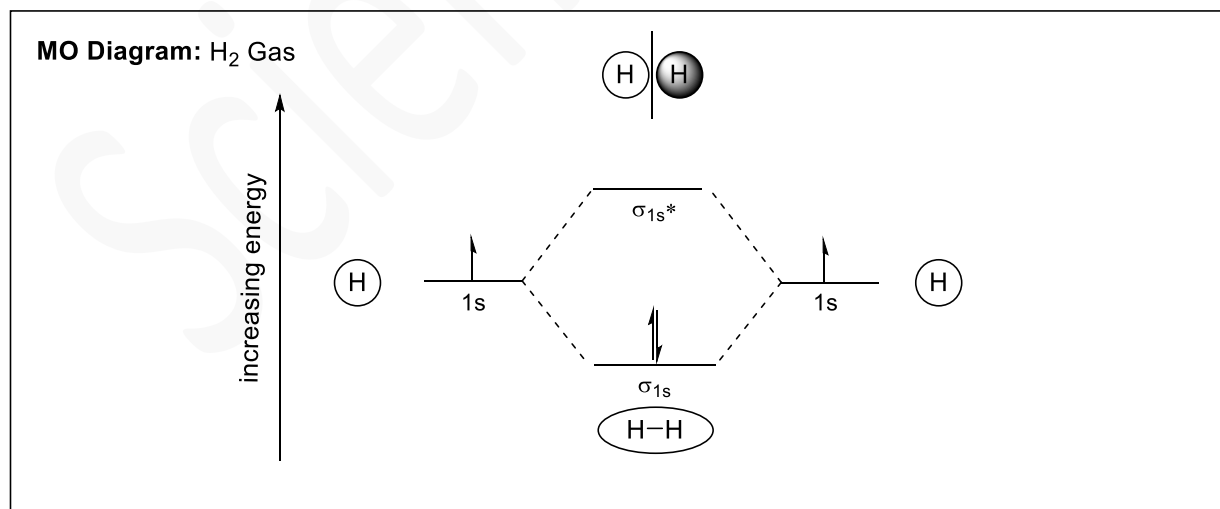


**IV. Molecular orbital (MO) theory** provides a quantum-mechanical explanation to bonding: covalent bonds are formed when atomic orbitals combine to create molecular orbitals. We will use the MO diagram for the formation of  $H_2$  gas to review the principles of MO theory.

- a. If we imagine the atomic s-orbital that each hydrogen brings to bonding, we see that two atomic orbitals are combining to form the  $H_2$  gas. When atomic orbitals combine to form bonds, the number of orbitals is conserved, and two new molecular orbitals are formed.
  - i. Of the two molecular orbitals created, one will be a lower energy bonding orbital and the other will be a higher energy anti-bonding orbital.
  - ii. Anti-bonding orbitals are indicated through misaligned phases or shading. The point of interference is termed a node.



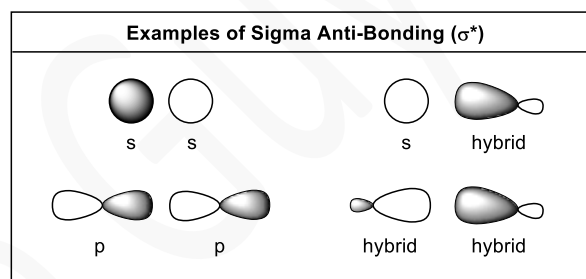
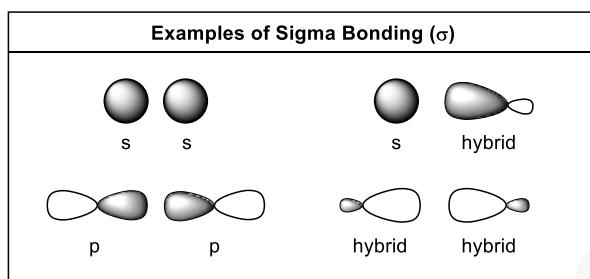
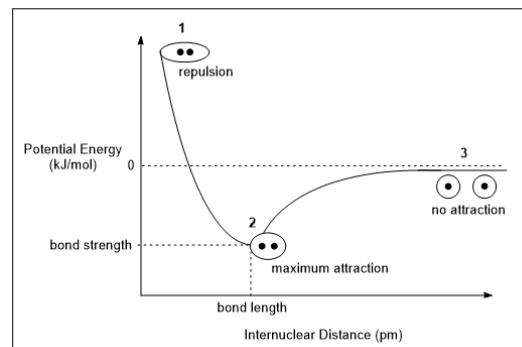
- b. If we plot the relative energy levels of the atomic and molecular orbitals, we create an MO diagram. Notice that the bonding MO is spin-paired, while the anti-bonding orbital is not. Since the anti-bonding orbital is not filled, we know that  $H_2$  can exist as a stable molecule.
  - i. **Highest occupied molecular orbital (HOMO):** represents the highest energy molecular orbital where electrons can be found.
  - ii. **Lowest Unoccupied Molecular Orbital (LUMO):** represents the lowest energy molecular orbital where electrons are not present.



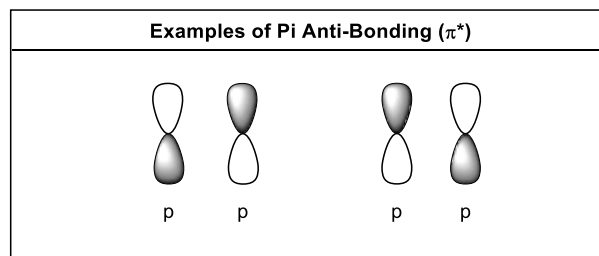
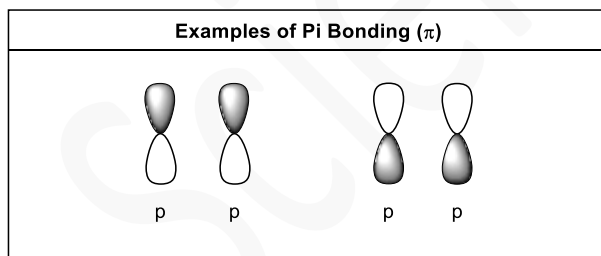
**Example:** Why doesn't helium exist as a diatomic  $He_2$  like hydrogen does?

V. **Valence bond (VB) theory** offers a simplified view of bond-formation: a covalent bond forms when two atoms reach an ideal bond length, and an orbital with one electron from each atom overlaps. This theory allows us to visualize the difference between sigma ( $\sigma$ ) and pi ( $\pi$ ) bonding according to orbital alignment.

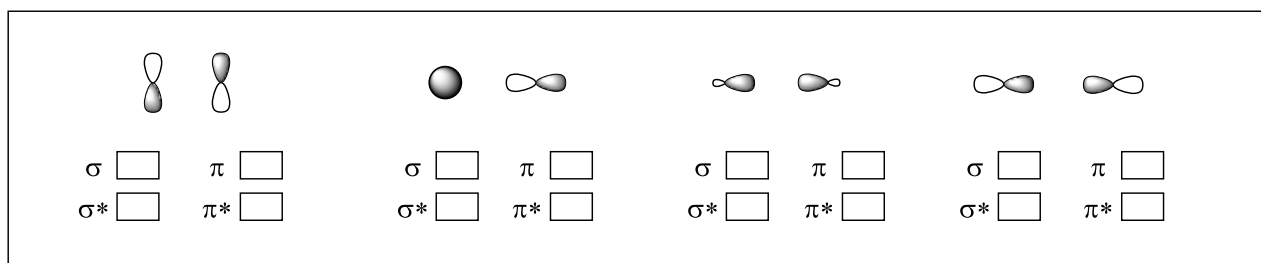
- Sigma bonding:** head-to-head overlap that results in single bonds. Remember, this can occur between two hybrid orbitals, an unhybridized orbital and a hybrid orbital, or two unhybridized orbitals.
- Sigma anti-bonding:** Form when valent orbitals overlap head-on and out-of-phase (opposite shading).



- Pi Bonding:** side-to-side overlap that results in double or triple bonds. Form when valent p orbitals overlap vertically and in-phase (same shading). Pi bonds can only be formed from p orbitals!
- Pi Anti-Bonding:** Form when valent p orbitals overlap vertically and out-of-phase (opposite shading).



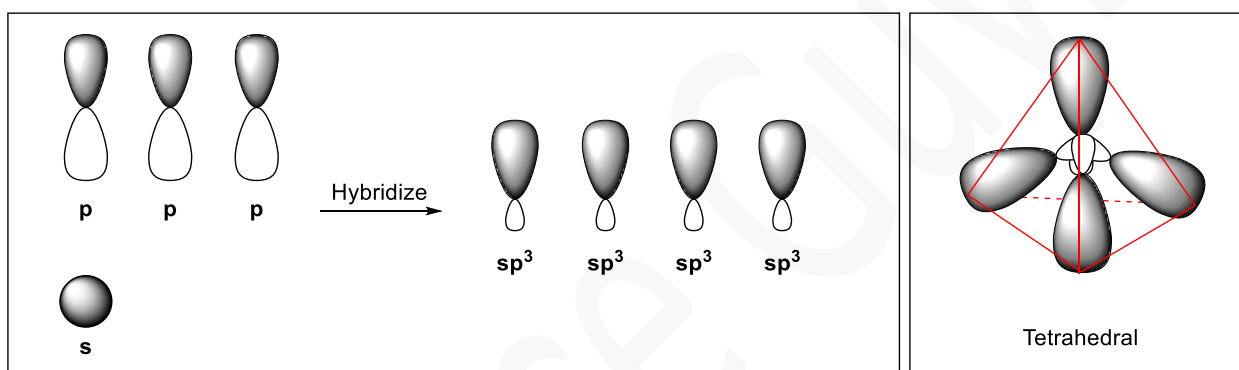
**Example:** Determine the type of bond that is being made by the two indicated orbitals when they overlap.



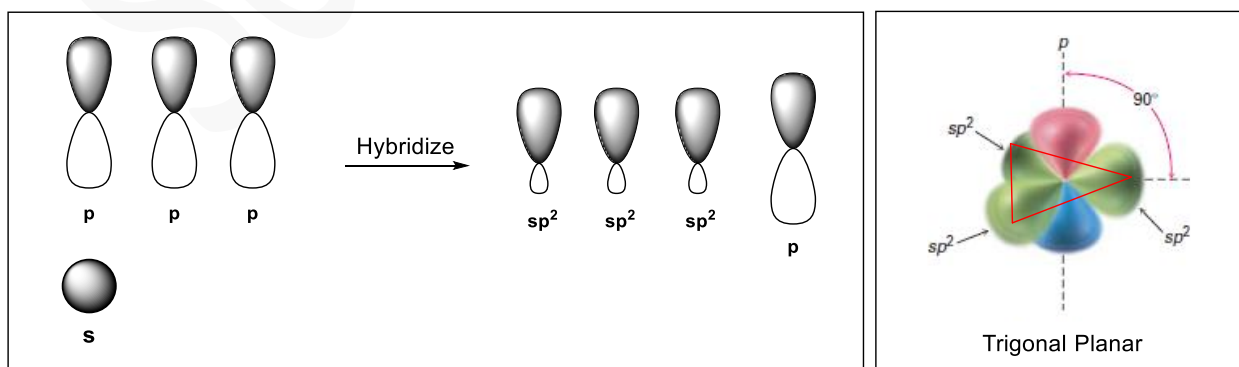
## Hybridization of Atomic Orbitals

I. **Hybridized orbitals** form when an atom (aside from hydrogen) prepares to bond, with atomic orbitals combining to create new orbitals that are more effective for bonding. In this discussion, we will focus on the hybridization resulting from the mixing of valent s- and p-orbitals.

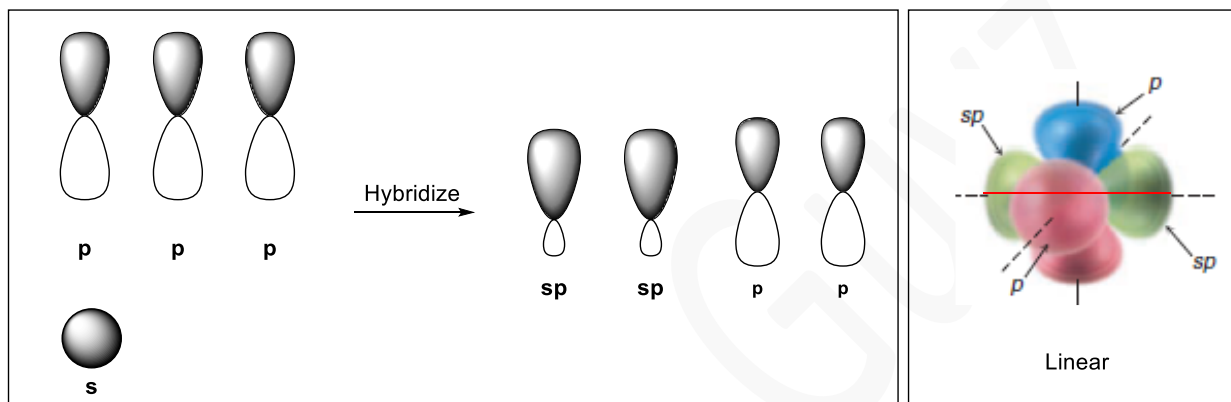
- a.  **$sp^3$  Hybridization:** Arises upon the mixing of one s- with three p-orbitals to form four degenerate  $sp^3$  orbitals.
  - i.  **$sp^3$  Electronic Geometry:** Termed tetrahedral, this can be understood by visualizing the four  $sp^3$  orbitals arranged around a central point, positioned to be as far apart as possible, resulting in a tetrahedral shape.
  - ii.  **$sp^3$  Ideal Bond Angles:** The angles between the vertices of a tetrahedron, measured from the center, are  $109.5^\circ$ . Note that the presence of lone pairs will reduce this angle.



- b.  **$sp^2$  Hybridization:** Arises upon the mixing of one s- with two p-orbitals to form three degenerate  $sp^2$  orbitals, leaving behind one non-hybridized p-orbital.
  - i.  **$sp^2$  Electronic Geometry:** Termed trigonal planar, this can be understood by visualizing the three  $sp^2$  orbitals arranged around a central point, positioned to be as far apart as possible, forming a trigonal shape. **Note:** The non-hybridized p-orbital must be oriented perpendicular to the plane of the hybrid orbitals.
  - ii.  **$sp^2$  Ideal Bond Angles:** The angles at two vertices of an equilateral triangle, measured from the center, correspond to  $120^\circ$ . Note that the presence of lone pairs will reduce this angle.



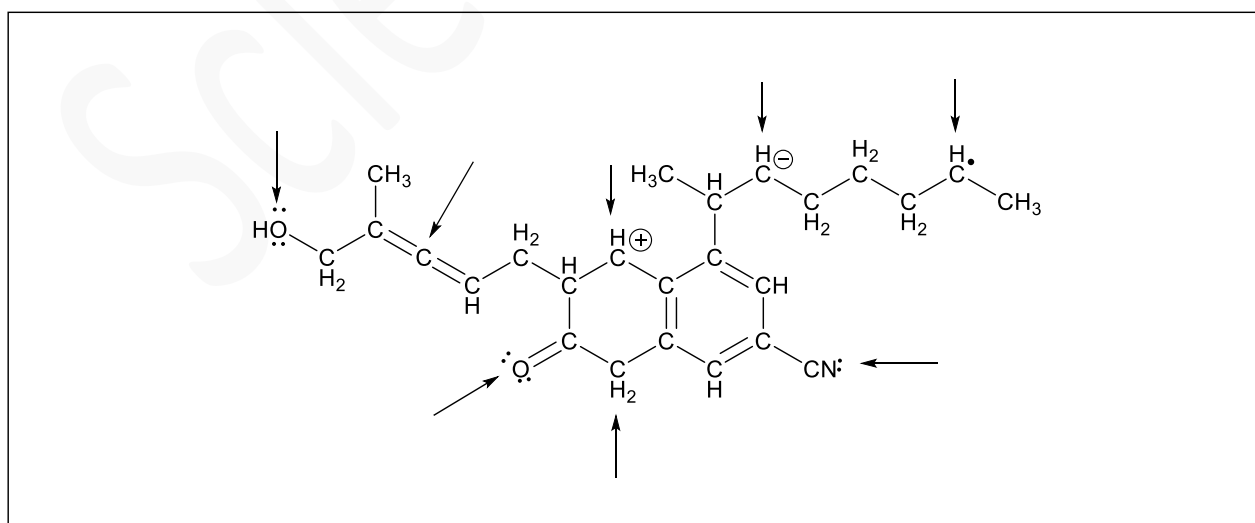
- c. **sp Hybridization:** Arises upon the mixing of one s- with one p-orbital to form two degenerate sp orbitals, leaving behind two non-hybridized p-orbitals.
- sp Electronic Geometry:** Termed linear, this can be understood by visualizing the two sp orbitals arranged around a central point, positioned to be as far apart as possible, resulting in a line. **Note:** The non-hybridized p-orbitals must be oriented perpendicular to the plane of the hybrid orbitals
  - sp Ideal Bond Angles:** The angles of two vertices of a line about the center of the line correspond to 180°. Note that the presence of lone pairs will reduce this angle.



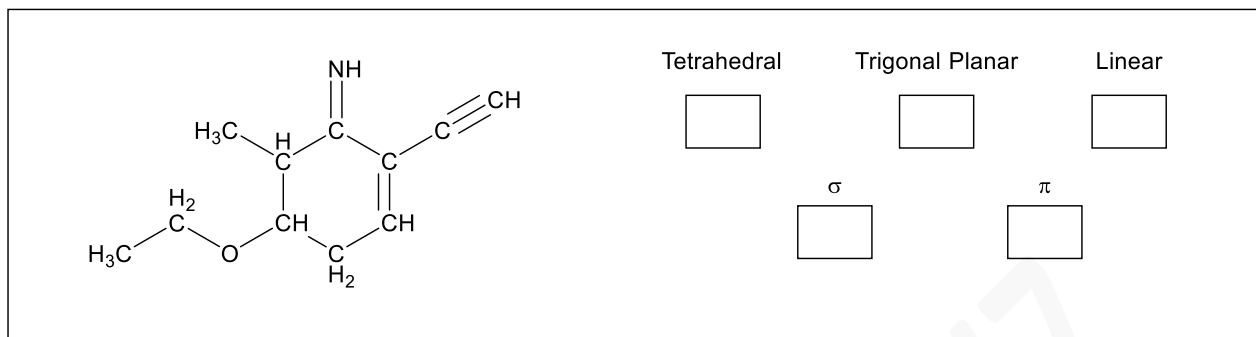
- V. The hybridization of an atom within a molecule is determined by summing its regions of electron density, which are areas where electrons are found. A region of electron density can be a lone pair, a single bond, a double bond, or a triple bond. Note that single electrons (radicals) are not counted as a region of electron density.

Regions of Electron Density	Hybridization
2	sp
3	sp <sup>2</sup>
4	sp <sup>3</sup>

**Example:** Determine the hybridizations on the atoms indicated below.



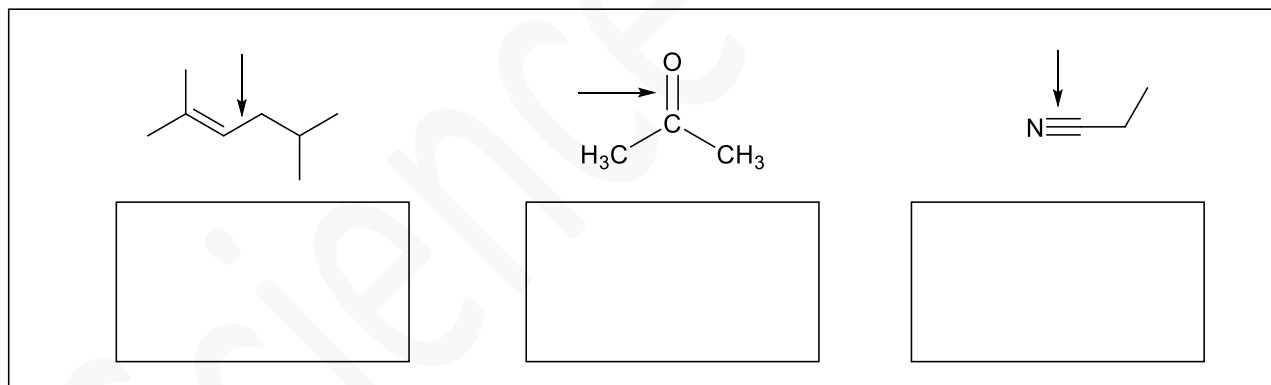
**Example:** Given the molecule below, provide the number of atoms with the corresponding electronic geometry in the boxes below. Additionally, indicate how many sigma and pi bonds are present.



**VI.** The orbital composition of a bond is determined by the bond type and the hybridization of the atoms involved.

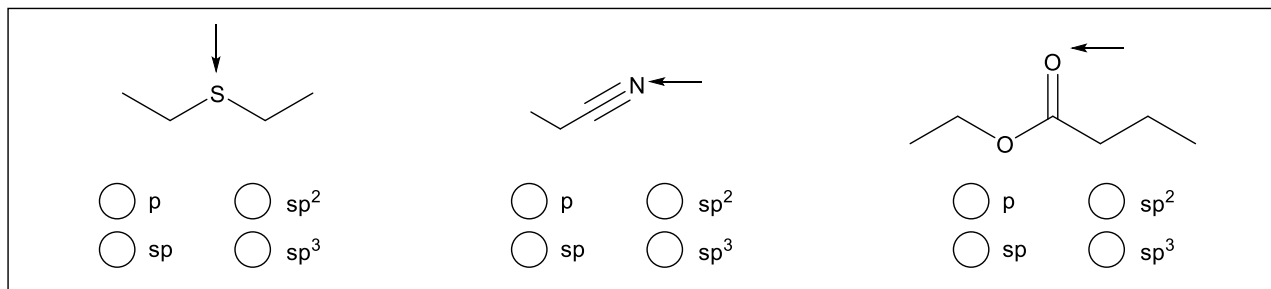
- Sigma bonds form from the overlap of hybrid orbitals or a hybridized orbital and an unhybridized s-orbital (as in hydrogen). To determine the composition of a sigma bond, identify the hybridization of the two atoms involved.
- Pi bonds form from the overlap of p-orbitals and the composition will always be two p-orbitals overlapping.

**Example:** Determine which orbitals overlap to form the indicated bonds in the compounds below.



**VII.** Lone pairs are typically located in hybrid orbitals, unless they can participate in resonance, in which case they occupy p-orbitals. We will revisit resonance in a later section.

**Example:** Determine which orbital the lone pair(s) on the following atoms are likely to be found in.

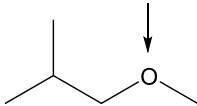
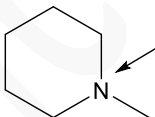
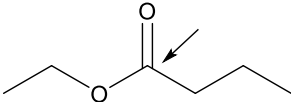


**VIII. The Valence-Shell Electron-Pair Repulsion (VSEPR) theory** builds upon hybridization by considering the influence of lone pairs on *molecular* geometry. The central idea of this theory is that both bonds and lone pairs strive to maximize their separation, minimizing electron pair repulsion.

- a. **Electronic geometry** considers all regions of electron density without distinguishing between bonding and non-bonding electrons, while **molecular geometry** accounts for both bonding and non-bonding electrons, with lone pairs influencing the overall molecular shape.

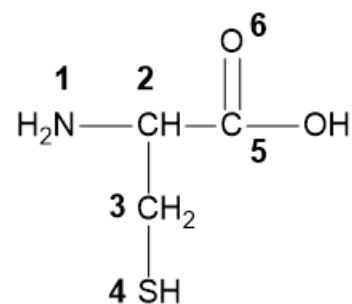
Regions of Electron Density	Hybridization	Lone Pairs of Electrons	Electronic Geometry	Molecular Geometry	Angles
2	sp	0	Linear	Linear	180°
3	sp <sup>2</sup>	0	Trigonal Planar	Trigonal Planar	120°
		1		Bent	< 120°
4	sp <sup>3</sup>	0	Tetrahedral	Tetrahedral	109.5°
		1		Trigonal Pyramidal	107°
		2		Bent	105°

**Example:** What is the predicted molecular geometry of the indicated atoms in the compounds below?

		
<input type="radio"/> Tetrahedral	<input type="radio"/> Tetrahedral	<input type="radio"/> Tetrahedral
<input type="radio"/> Trigonal Planar	<input type="radio"/> Trigonal Planar	<input type="radio"/> Trigonal Planar
<input type="radio"/> Trigonal Pyramidal	<input type="radio"/> Trigonal Pyramidal	<input type="radio"/> Trigonal Pyramidal
<input type="radio"/> Bent	<input type="radio"/> Bent	<input type="radio"/> Bent

**Example:** Answer the following questions about the amino acid cysteine shown below.

- (True/False) The electronic geometry of atoms 1, 2, 3 & 4 are tetrahedral.
- (True/False) The molecular geometry of atoms 1, 2, 3 & 4 are tetrahedral.
- (True/False) The sigma bond between atoms 2 & 5 is formed from sp<sup>2</sup>-sp<sup>2</sup> overlap.
- (True/False) There are 6 sigma bonds present.
- (True/False) The lone pair on atom 1 occupies an sp<sup>3</sup> orbital.
- (True/False) The bond angle of the 2-3-4 bond is ~110°.



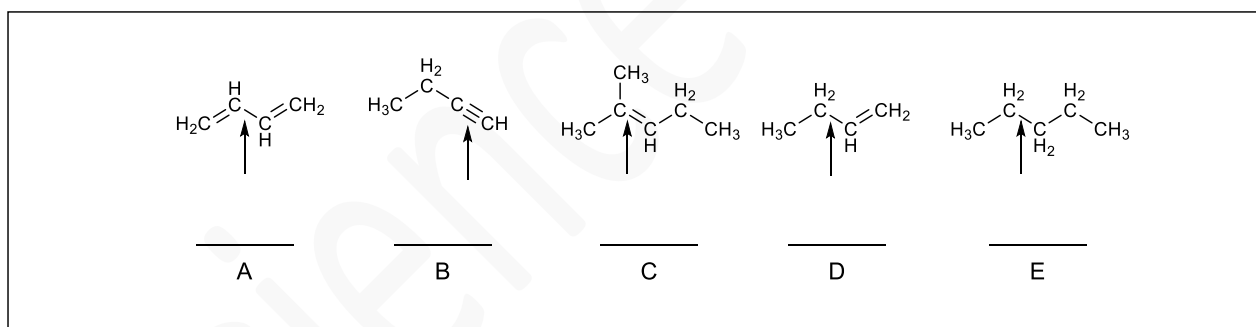


**Bond Length & Bond Strength:**

- I. **Pi Bonds Effect on Bond Strength:** Generally, triple bonds are shorter and stronger than double bonds. Double bonds are shorter and stronger than single bonds. When comparing two bonds of the same type, the shorter/stronger bond will be the bond that has the most s-character.

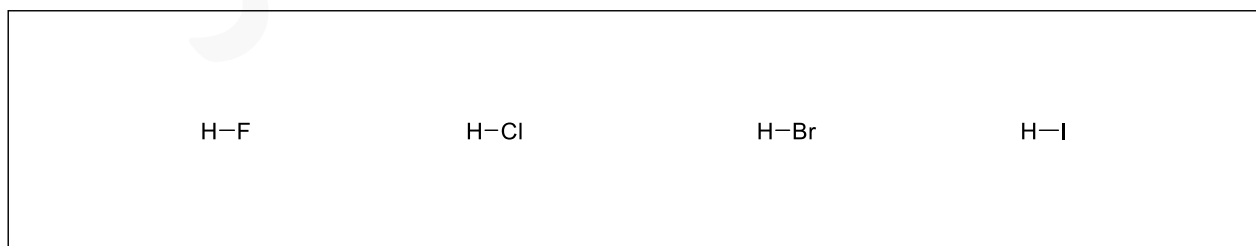
Increasing s-character ↑	Increasing bond strength ↑	Decreasing bond length ↓
$\% \text{ s-character} = \frac{\text{number of s orbitals}}{(\text{number of s orbitals} + \text{number of p orbitals})} \times 100$		
<u>        </u> sp <sup>3</sup>	<u>        </u> sp <sup>2</sup>	<u>        </u> sp

**Example:** Rank the indicated bonds from longest to shortest (1 = longest).



- II. **The Hydrogen Halides:** the bigger the halogen, the longer the bond be to the hydrogen. The longer the bond, the weaker it will be.

**Example:** Of the hydrogen halides, which has the strongest H-X bond? Which has the longest?



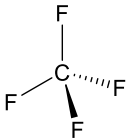
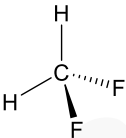
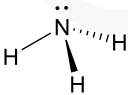
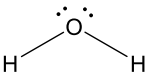
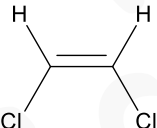
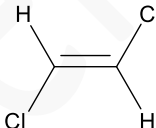
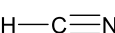
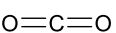
**Dipole Moments and Molecular Polarity:**

- I. **Dipole Moment ( $\mu$ ):** an indicator of polarity; occurs in polar bonds when there is sufficient distance between opposing charges. The exact dipole moment of a bond can be calculated using the formula below:

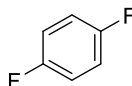


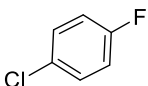
$$\text{Dipole moment } \mu = (\text{size of the charge } \delta) \times (\text{distance between the charges } d)$$

- II. **Molecular dipole moment** represents the sum of all dipole moments in a molecule with more than one polar bond. Due to the molecular geometry of molecules, it is possible for dipole moments to cancel each other out and make a molecule non-polar overall.
- Non-polar molecules** contain only non-polar bonds or contains polar bonds in equal and opposite directions.
  - Polar molecules** contain polar bonds that are not evenly distributed.

**Example:** Determine if the molecules shown below are polar or non-polar.

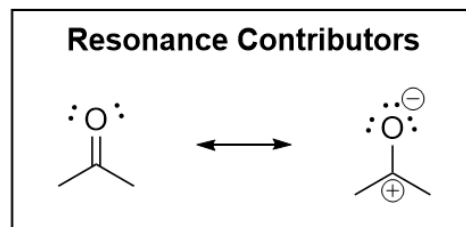
			
<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar
			
<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar	<input type="checkbox"/> Polar <input type="checkbox"/> Non-Polar

**Example:** Rank the following molecules in order of increasing overall dipole moment (4 = highest).

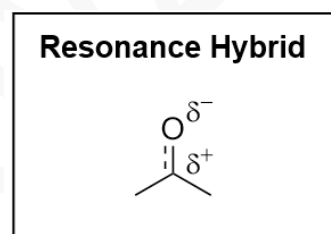
			
A	B	C	D

## Resonance

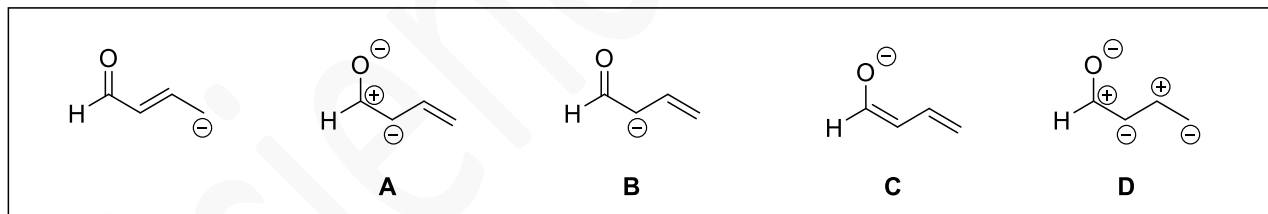
- I. **Resonance** involves the delocalization of pi electrons (those in double or triple bonds) and non-bonding electrons (such as lone pairs or radicals), leading to a distribution of electron density across a molecule that enhances its stability.
- II. **Resonance contributors** are structures that share the same molecular formula, connectivity, and sigma backbone, but differ in the placement of pi electrons. These contributors show the possible ways electron density can be distributed, and while some can be more stable than others, none of them fully represent the true molecule.
- III. The actual structure of a resonating molecule is known as the **resonance hybrid**, which is an average of all resonance contributors, reflecting the delocalized nature of the electron density.



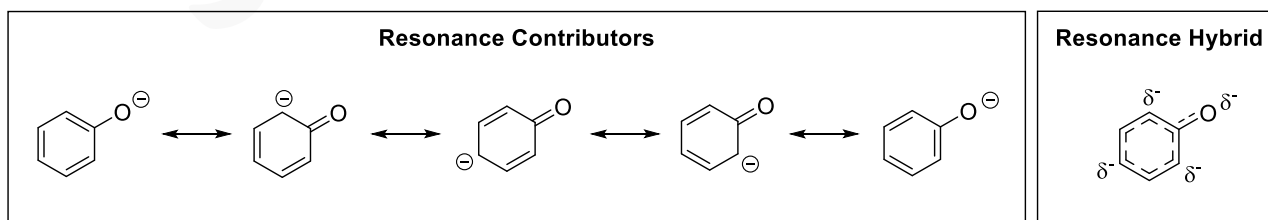
- a. Not all resonance contributors contribute equally to the hybrid; the most stable contributor has octets on all atoms, with the negative charge on the more electronegative atom.
  - i. If octets can't be achieved, the most significant contributor places the positive charge on the more electropositive atom.
  - ii. Resonance forms that introduce more separation of charges relative to other structures are generally considered minor contributors.



**Example:** Given the four possible resonance forms below, which contributor would you expect to be the major contributor? Which do you think contributes the least?

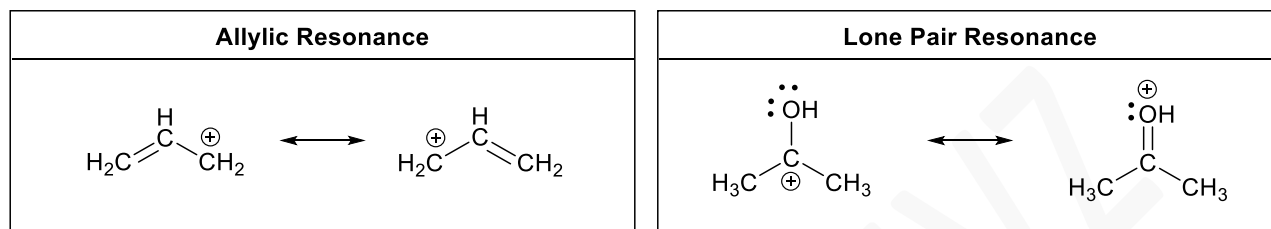


- b. Resonance hybrids are assembled by drawing a dotted line over the system of pi electrons and/or lone pairs that you moved to create each individual resonance structure. Wherever formal charges appeared in the contributors, the hybrid will feature a partial ( $\delta$ ) charge.

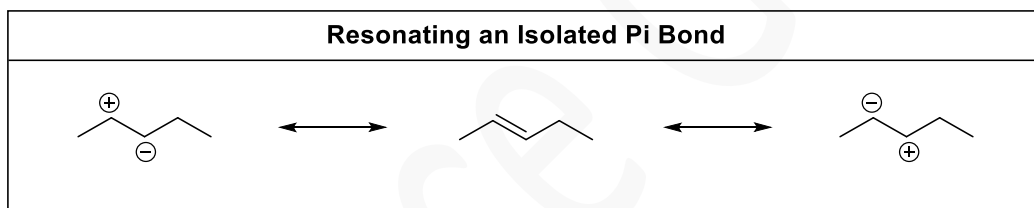


- IV. **Beware:** Resonance can cause the true hybridization of an atom to be different than the apparent hybridization of the atom. An atom must be  $sp^2$  or  $sp$  to participate in resonance.

- V. There are two main types of resonance we will encounter in this course: allylic resonance and lone pair resonance.
- Allylic resonance occurs when a cation, anion, lone pair, or radical is located adjacent to a pi bond. This is termed the **allylic** position.
  - Lone pair resonance occurs when the lone pairs on an atom, such as oxygen or nitrogen, can participate in resonance by sharing a lone pair with an adjacent electron-deficient atom.

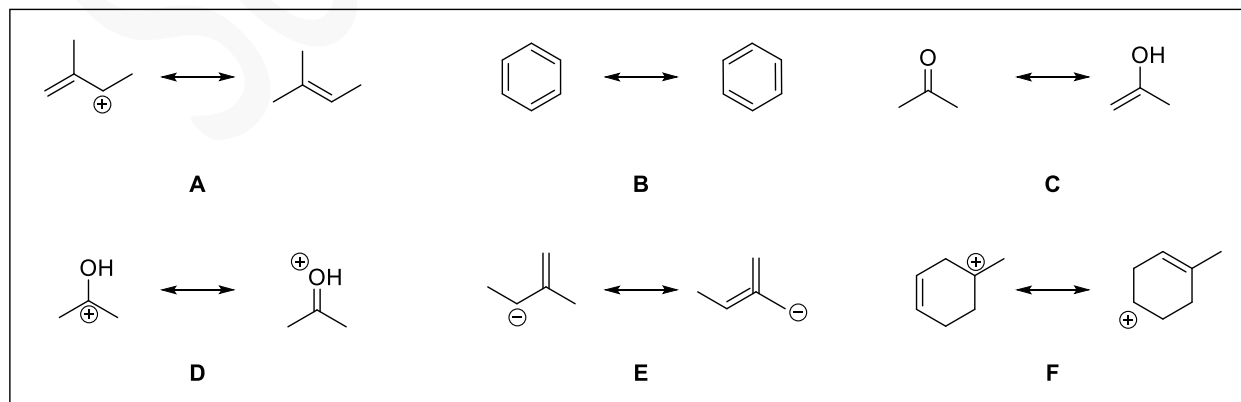


- A less favorable, but still possible, resonance type involves resonating isolated pi bonds to introduce a separation of charges. This type of resonance is always possible if a pi bond is present, but generally, isn't considered a major contributor due to charge separation.



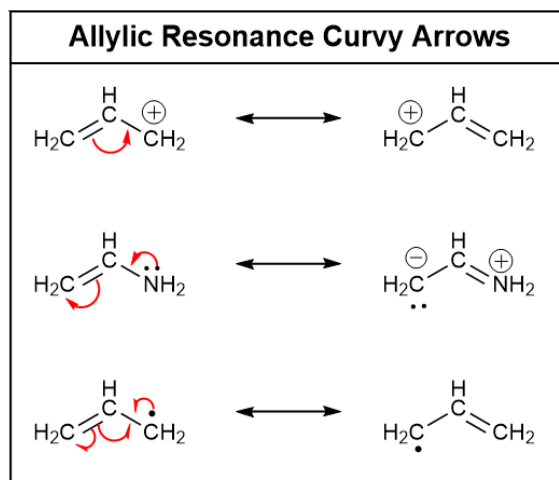
- VI. **Rules of Resonance:** When resonating a compound, there are some rules to keep in mind:
- The net charge of the molecule must remain constant. For two forms to be considered resonance forms, the net charge on the compound must remain constant between them.
  - Never break sigma (single) bonds, only pi bonds and pi electrons can move.
  - Do not violate the octet rule. Be mindful of this rule and its exceptions as you are proposing resonance structures.

**Example:** Which of the following represents a valid pair of resonance structures? Select all that apply.

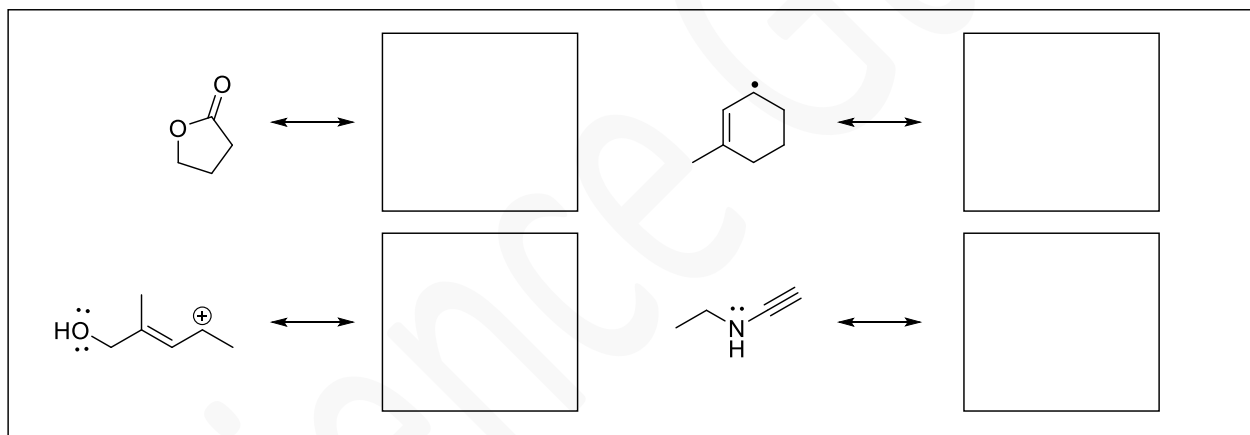


VII. **Allylic resonance** can be shown using curly arrows, where the number of arrows depends on the type of resonance occurring.

- Allylic cation:** requires one double-headed curly arrow from pi bond to single bond.
- Allylic lone pair/anion:** requires two double-headed curly arrows. The first from the lone pair/anion to the single bond, and the second from the pi bond to the next atom.
- Allylic radical:** requires three single-headed arrows. The first from the radical to the single bond, the second from the pi bond to meet the other arrow at the single bond, the third to place the remaining electron on the next atom.

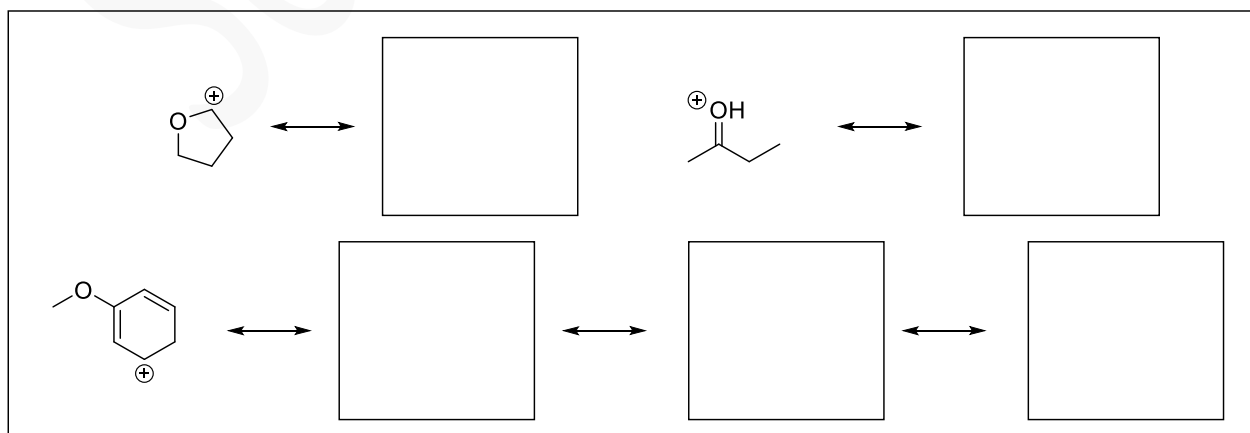


**Example:** Provide resonance forms for the following compounds, including curly arrows.

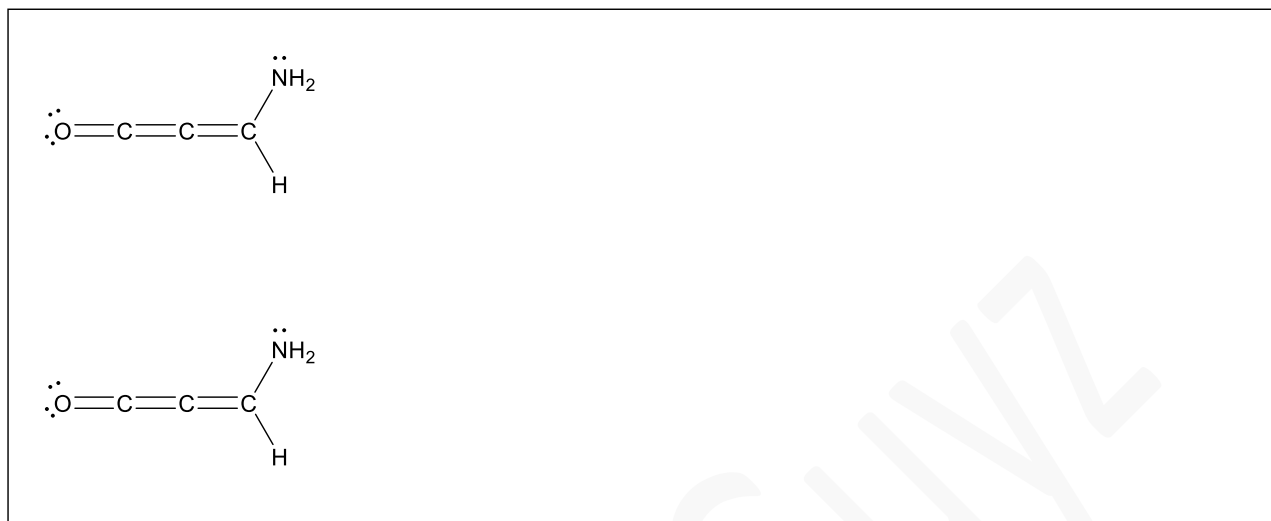


VIII. **Lone pair resonance** generally requires one curly arrow pointed from the lone pair to the adjacent single bond.

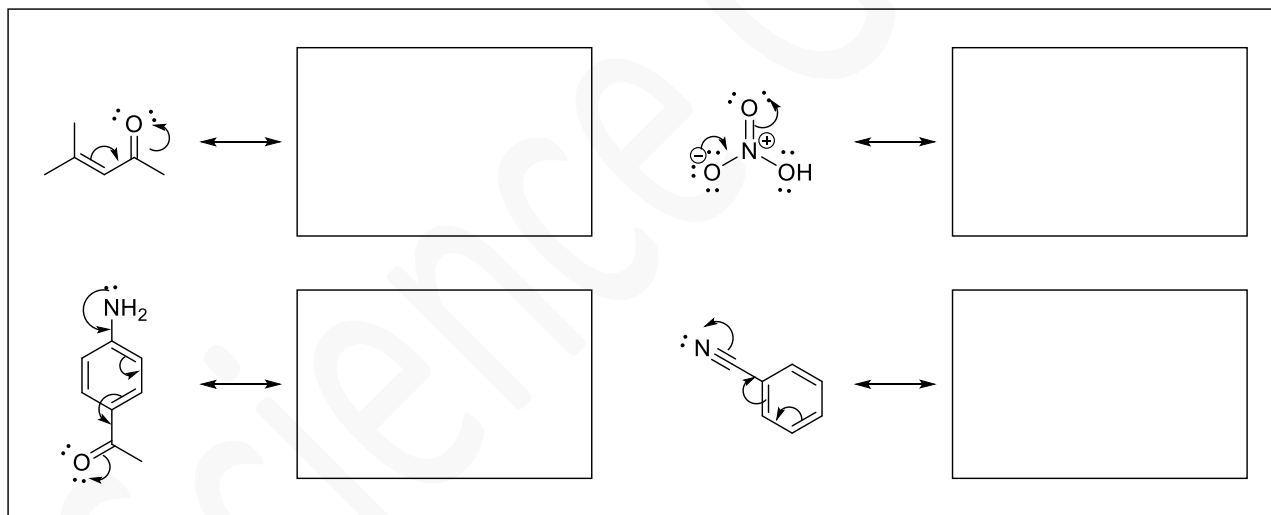
**Example:** Provide resonance forms for the following compounds, including curly arrows.



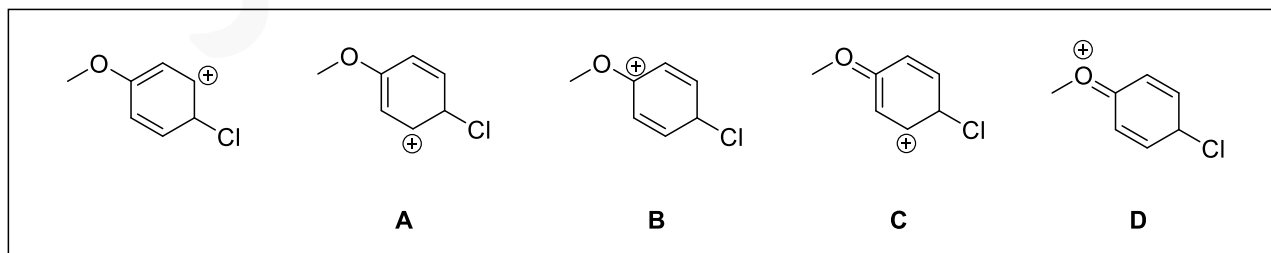
**Example:** The structure below has two lone pairs capable of delocalization. Which lone pair can be delocalized more than the other?



**Example:** Draw the structure that results from the resonance arrows shown below.



**Example:** Given the molecule below, predict which of the shown molecules is NOT a resonance contributor as defined by the others.



**Essential Concepts Cheat Sheet:****Drawing Lewis Structures**

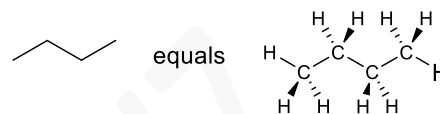
1. Sum the valence electrons. (anions +1, cations -1)
2. Determine central atom.
3. Add valence electrons to central atom.
4. Connect surrounding atoms via covalent bonds.
5. Insert pi bonds if needed.
6. Assign formal charges.  $FC = (\# \text{ val } e^-) - (\# \text{ dots}) - (\# \text{ lines})$

**Preferred Bonding Arrangements**

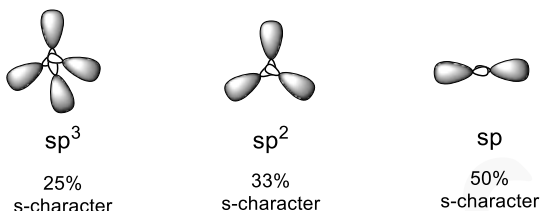
	C	N	O	F
# lone pairs	0	1	2	3
# bonds	4	3	2	1

**Determining Hybridization**

Regions of E <sup>-</sup> Density	Hybridization	Electronic Geometry	Ideal Bond Angles
2	sp	Linear	180°
3	sp <sup>2</sup>	Trigonal Planar	120°
4	sp <sup>3</sup>	Tetrahedral	109.5°

**Skeletal/Bond Line Structure****Bond Composition**

C≡C	C=C	C-C
1 sigma 2 pi	1 sigma 1 pi	1 sigma

**Hybridized Atomic Orbitals**

↑ s-character = ↓ bond length and ↑ bond strength

↑ atomic radii = ↑ bond length and ↓ bond strength

**Bonding Between Orbitals (orbital overlap)**

σ (sigma):  
head-to-head,  
in-phase



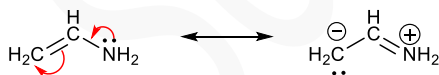
σ\* (sigma anti):  
head-to-head,  
out-of-phase



π (pi):  
vertical overlap,  
in-phase



π\* (pi anti):  
vertical overlap,  
out-of-phase

**Allylic Resonance Curvy Arrows****Most Contributing Resonance Form**

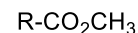
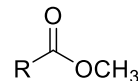
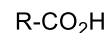
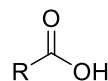
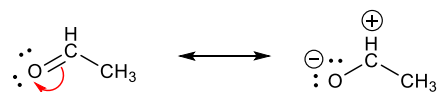
- all atoms have an octet
- negative charge on most electronegative atom

**Resonance Hybrid**

- dotted lines where all pi bonds appeared
- partial charges wherever full charges appeared

**Condensed Shorthands**

R = rest of molecule

**Lone Pair Resonance Curvy Arrows**

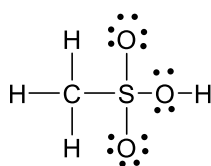
**Practice Set:** Test your understanding and complete the following problems! The key can be found on the Semester Plan playlist.

**Section:** Lewis Structures

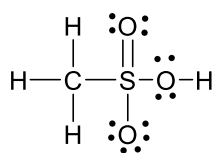
1. Draw a valid Lewis structure of the formula  $\text{CH}_2\text{O}$ .

2. Draw a valid Lewis structure of the formula  $\text{C}_6\text{H}_6$ .

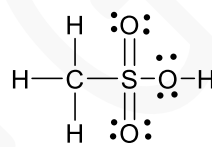
3. Which of the following is the most favored Lewis structure of  $\text{CH}_3\text{SO}_3\text{H}$ ?



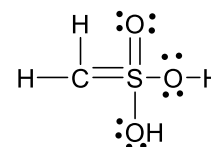
**A**



**B**

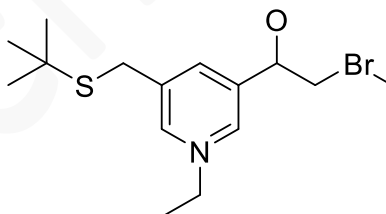


**C**

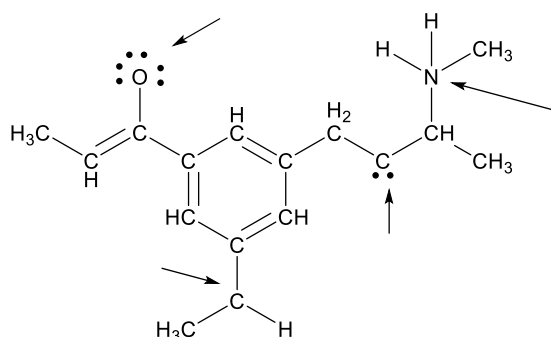


**D**

4. How many heteroatoms in the structure below have a non-zero formal charge? Assume they each have a full octet.

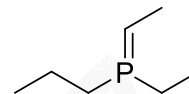
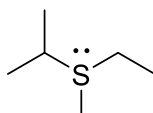
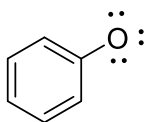
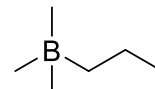
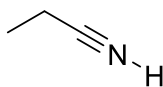
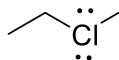


5. Provide the formal charge on the atoms indicated below. All electrons have been shown.



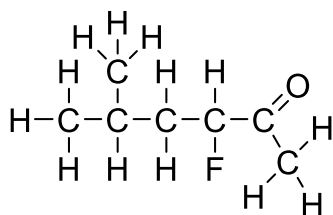


6. Provide the formal charge on the heteroatoms indicated below. All electrons have been shown.



**Section:** Drawing Structural Representations

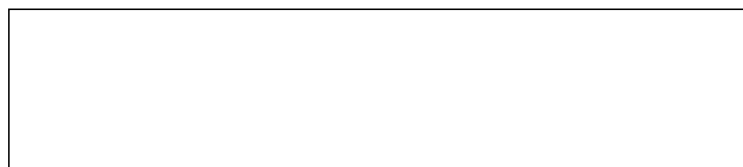
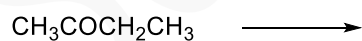
7. Convert the following Kekulé structure to condensed and skeletal structure.



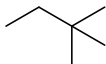
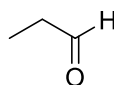
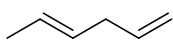
8. Convert the following condensed structures to skeletal structures.

**Condensed**

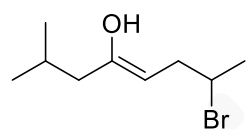
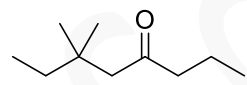
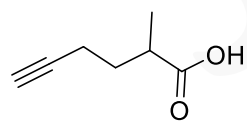
**Skeletal**



9. Convert the following skeletal structures to Kekulé structures.

<u>Skeletal</u>	→	<u>Kekulé</u>
	→	
	→	
	→	

10. Convert the following skeletal structures to condensed structures.

<u>Skeletal</u>	→	<u>Condensed</u>
	→	
	→	
	→	

**Section:** Hybridization & Orbital Overlap

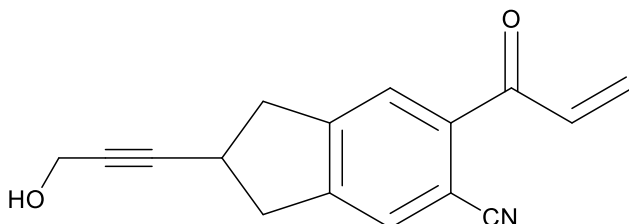
11. Which of the atomic orbital combinations shown below will result in a sigma molecular orbital?



12. Which of the atomic orbital combinations shown below will result in a  $\pi^*$  molecular orbital?

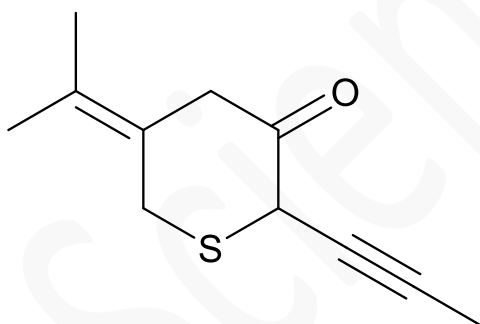


13. For the compound given below, provide the molecular formula. Additionally, provide the number of sigma and pi bonds. Finally, determine the number of  $sp$ ,  $sp^2$  and  $sp^3$  hybridized atoms.



<b>Sigma Bonds</b>	<b>Pi Bonds</b>	<b><math>sp</math> hybridized atoms</b>	<b><math>sp^2</math> hybridized atoms</b>	<b><math>sp^3</math> hybridized atoms</b>
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

14. For the compound given below, indicate the number of atoms with the indicated geometries. Additionally, indicate the number of methylene groups present. Lastly, circle the most polar bond in the compound.



Tetrahedral Atoms:

Trigonal Planar Atoms:

Linear Atoms:

Methylene:

15. In what orbital does the lone pair reside in for a methyl anion ( $\text{CH}_3^-$ )?

16. What orbitals are used to form the C-O bond in ethanol ( $\text{CH}_3\text{CH}_2\text{OH}$ )?

17. What orbitals are used to form the C=O bond in acetone ( $\text{CH}_3)_2\text{CO}$ )?

**Section: Bond Length & Bond Strength**

18. Rank the indicated bonds in order of increasing strength (4 = strongest).



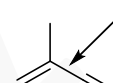
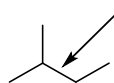
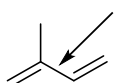
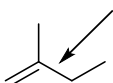
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19. Rank the indicated bonds in order of decreasing length (1 = longest).



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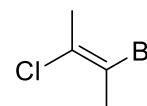
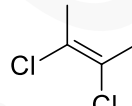
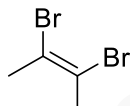
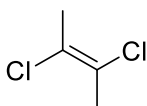
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**Section: Dipole Moments and Molecular Polarity**

20. Rank the following compounds in order of increasing polarity (1 = most polar).



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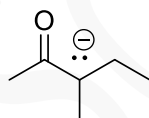
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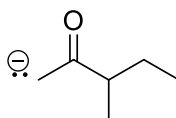
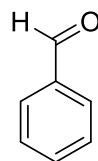
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**Section: Resonance**

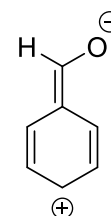
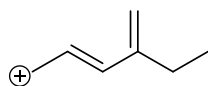
21. Which of the pairs of compounds below represent resonance forms?



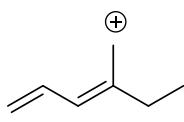
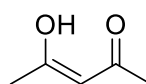
and

**A**

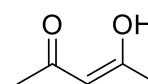
and

**B**

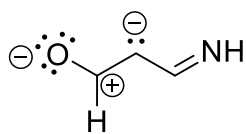
and

**C**

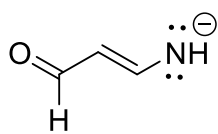
and

**D**

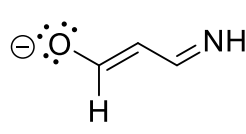
22. Which resonance form below is the most contributing?



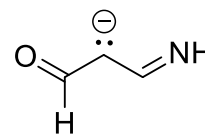
A



B



C

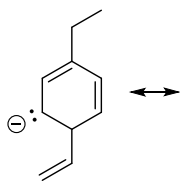


D

23. Provide all resonance forms the compound below. Additionally, provide the resonance hybrid.

Resonance Forms

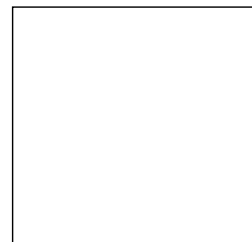
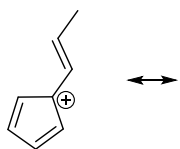
Resonance Hybrid



24. Provide all resonance forms the compound below. Additionally, provide the resonance hybrid.

Resonance Forms

Resonance Hybrid



25. Provide all resonance forms the compound below. Additionally, provide the resonance hybrid.

Resonance Forms

Resonance Hybrid

