



ScienceGuyz

CHEM 2211

Chapter 1:

Atomic Structure and Hybridization

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Spring 2022

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Introduction:

Welcome to Organic Chemistry! In this course, we are primarily concerned with organic compounds, or compounds that are based on carbon. Life itself is composed of carbon-based compounds and many concepts that you will learn in this course can help explain principles in other courses you may take, including biology, biochemistry, and genetics. In this chapter, we will be reviewing concepts from general chemistry that will serve as the foundation for your organic chemistry learning.

Learning Objectives: By the end of this workshop, you should be able to:

- Describe the difference between ionic and covalent bonds.
- Identify polar and non-polar bonds or molecules.
- Rank molecules according to their relative dipole moment.
- Draw various structure representations, such as Lewis, condensed and skeletal.
- Determine the hybridization, molecular geometry, and ideal bonding angles of an atom.
- Indicate which atoms lie in the same plane as an sp^2 hybridized atom.
- Calculate the formal charge of an atom.
- Describe bond composition.
- Differentiate between bonding and anti-bonding in orbitals.
- Differentiate between a sigma bond and a pi bond.
- Predict relative bond strengths.
- Draw all resonance structures and a resonance hybrid for a molecule.
- Depict electron movement with single-headed and double-headed arrows.

The Basics:

- I. An atom is composed of a nucleus surrounded by an electron cloud.
- II. The nucleus contains positively charged protons and uncharged neutrons.
- III. The electron cloud is composed of negatively charged electrons.
- IV. The chemical behavior of an atom depends on the number of valence electrons that atom has. In organic chemistry, we are primarily concerned with the atoms outermost shell of electrons because those are the electrons involved in bonding.
- V. Life works towards becoming more stable. More stability means lower energy, which makes a compound less reactive. This is the common theme in organic chemistry, as all molecules work towards becoming more stable.

1 H 1.008																	2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.81	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.06	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.88	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.63	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.94	43 Tc 98.906	44 Ru 101.07	45 Rh 101.07	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.6	53 I 126.905	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57-70 * Lu 174.967	71 Hf 178.49	72 Ta 180.948	73 W 183.84	74 Re 186.207	75 Os 190.23	76 Ir 192.22	77 Pt 195.084	78 Au 196.967	79 Hg 200.59	80 Tl 204.38	81 Pb 207.2	82 Bi 208.98	83 Po 209	84 At 210	85 Rn 222
87 Fr 223	88 Ra 226	89-102 ** Lr 260	103 Rf 261	104 Db 262	105 Sg 263	106 Bh 264	107 Hs 265	108 Mt 266	109 Uun 267	110 Uuu 268	111 Uub 269	114 Uuq 269					

Bonding Between Atoms:

- I. **Ionic bonds** are generally formed when a metal is bound to a non-metal. The atoms form a bond through electrostatic interactions of their respective opposing charges. Arises when one atom completely gives its electrons to another atom forming two or more charged atoms. For ionic molecules, 100% ionization is assumed. Therefore, an absolute charge is placed on both atoms participating in the bond under analysis.
- II. **Covalent bonds** are formed when two non-metal atoms share electrons between them. Arises between atoms when the valent electronic orbitals of two atoms come sufficiently close that the two atoms participating in the covalent bond attract one another, ultimately sharing electrons between the two atomic nuclei.

Example: Determine if the shown bonds are ionic or covalent.

Na—Cl	H—CH ₃	Cl—MgCl	Li—CH ₃	H—Br
<input type="checkbox"/> Ionic				
<input type="checkbox"/> Covalent				

A Deeper Look into Covalent Bonding: Electronegativity and Polar Bonds:

- I. We just defined covalent bonds as a sharing of electrons between two atoms, but that sharing is not always equal. The electron distribution in the bond depends on the electronegativities of the atoms involved.
- II. **Electronegativity** is defined as the tendency of an atom participating in a covalent bond to pull electron density towards itself. This leads to an unequal sharing of electrons within the bond.

INCREASING ELECTRONEGATIVITY

← INCREASING ELECTRONEGATIVITY																		→														
1 H 1.024																	2 He 1.000	INCREASING ELECTRONEGATIVITY														
3 Li 0.978	4 Be 1.571															5 B 2.041	6 C 2.556		7 N 3.044	8 O 3.436	9 F 3.980	10 Ne 4.796										
11 Na 0.934	12 Mg 1.312															13 Al 1.511	14 Si 1.900		15 P 2.192	16 S 2.580	17 Cl 3.163	18 Ar 3.241										
19 K 0.822	20 Ca 0.930	21 Sc 1.360	22 Ti 1.545	23 V 1.633	24 Cr 1.631	25 Mn 1.551	26 Fe 1.830	27 Co 1.881	28 Ni 1.913	29 Cu 1.908	30 Zn 1.654	31 Ga 1.812	32 Ge 2.021	33 As 2.203	34 Se 2.550	35 Br 2.962	36 Kr 3.000															
37 Rb 0.822	38 Sr 0.950	39 Y 1.229	40 Zr 1.358	41 Nb 1.471	42 Mo 1.551	43 Tc 1.630	44 Ru 1.860	45 Rh 1.881	46 Pd 1.928	47 Ag 1.924	48 Cd 1.690	49 In 1.781	50 Sn 1.960	51 Sb 2.051	52 Te 2.100	53 I 2.496	54 Xe 2.600															
55 Cs 0.794	56 Ba 0.854	57 La 1.043	58 Ce 1.047	59 Pr 1.050	60 Nd 1.053	61 Pm 1.056	62 Sm 1.059	63 Eu 1.062	64 Gd 1.065	65 Tb 1.068	66 Dy 1.071	67 Ho 1.074	68 Er 1.077	69 Tm 1.080	70 Yb 1.083	71 Lu 1.086	72 Hf 1.380		73 Ta 1.480	74 W 1.580	75 Re 1.680	76 Os 1.780	77 Ir 1.880	78 Pt 1.980	79 Au 2.080	80 Hg 2.180	81 Tl 2.280	82 Pb 2.380	83 Bi 2.480	84 Po 2.580	85 At 2.680	86 Rn 2.780
87 Fr 0.700	88 Ra 0.700	89 Ac 0.700	90 Th 0.700	91 Pa 0.700	92 U 0.700	93 Np 0.700	94 Pu 0.700	95 Am 0.700	96 Cm 0.700	97 Bk 0.700	98 Cf 0.700	99 Es 0.700	100 Fm 0.700	101 Md 0.700	102 Ds 0.700	103 Nh 0.700	104 Fl 0.700		105 Mc 0.700	106 Lv 0.700	107 Ts 0.700	108 Og 0.700	109 Tennessine	110 Oganesson	111 Cn	112 Nh	113 Fl	114 Lv	115 Ts	116 Og	117 Tennessine	118 Oganesson

- III. **Polar bonds** are formed when there is an unequal sharing of electrons between two atoms participating in a covalent bond. However, if there is not a substantial difference in electronegativity between two atoms, that is known as a **nonpolar bond**.
- IV. **Dipoles** arise when electrons within a bond are not being shared equivalently. The total dipole moment of a compound is equal to the sum of all individual dipoles. They are often depicted using a vector that points to the more electronegative atom within the bond.
- V. **Dipole moments** refer to the intensity of the dipole and can be calculated by the equation shown below.

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

$$\mu = \delta \times d$$

Example: Given the following bonds shown below, first determine if the bond is polar or non-polar. If the bond is polar, indicate the direction of the dipole in the bond.


 Polar

 Non-polar

 Polar

 Non-polar

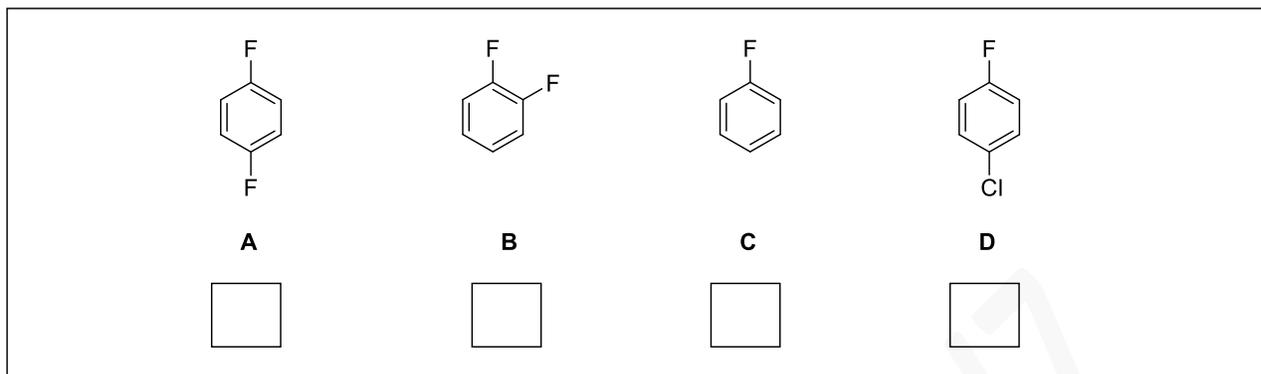
 Polar

 Non-polar

 Polar

 Non-polar

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



Structural Representations:

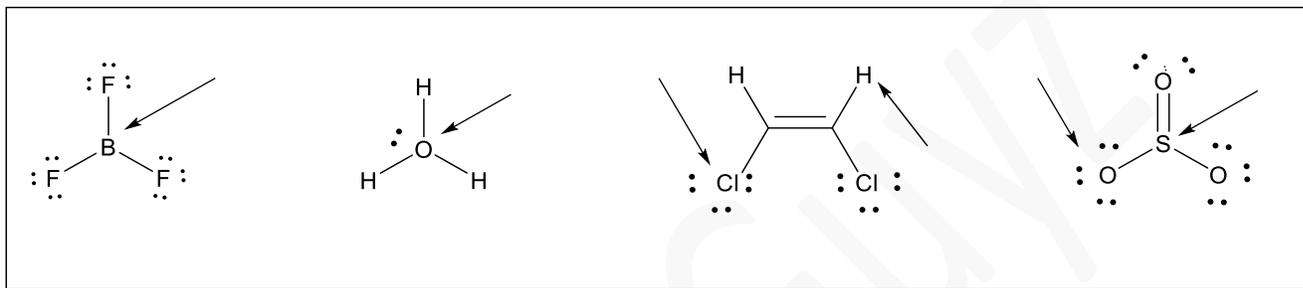
- I. **Lewis Structures:** structural representation of a molecule/atom/ion that shows all valence electrons and charges.
- II. **Steps for Drawing Lewis Structures:**
 - a. **Determine the total number of valence electrons.** Using the molecular formula, sum the total number of valence electrons present in the molecule. For non-neutral compounds (ions), adjust the total count:
 1. Anions (-): For each negative charge, add one electron.
 2. Cations (+): For each positive charge, subtract one electron.
 - b. **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.
 - c. **Add valence electrons to the central atom.** Add the number of valence electrons which the central atom has been designated to have based on the periodic chart, to the central atom.
 - d. **Connect atoms via covalent bonds.** Make bonds connecting the central atom to other atoms such that each atom gains an octet. The number of valent electrons present in the connecting atoms can be determined from the periodic chart as well.
 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
 - e. **Insert multiple bonds.** Double or triple bonds sometimes may be made in order to satisfy the octet rule. Insert these one at a time, as needed.
 - f. **Assign formal charges.** Assign formal charge to each atom in the structure that has a formal charge different than zero.
 - g. **Choose the favored structure.** Some formulas may yield multiple valid structures. The most favored structure will be the one that minimizes formal charges overall.

III. Formal Charge equates to the absolute charge that an atom within a molecule possesses, based on the molecule's Lewis Structure. Formal charge can be determined using the equation shown below:

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

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

Example: Determine the missing formal charges on the indicated atoms in the molecules shown below.



IV. 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.

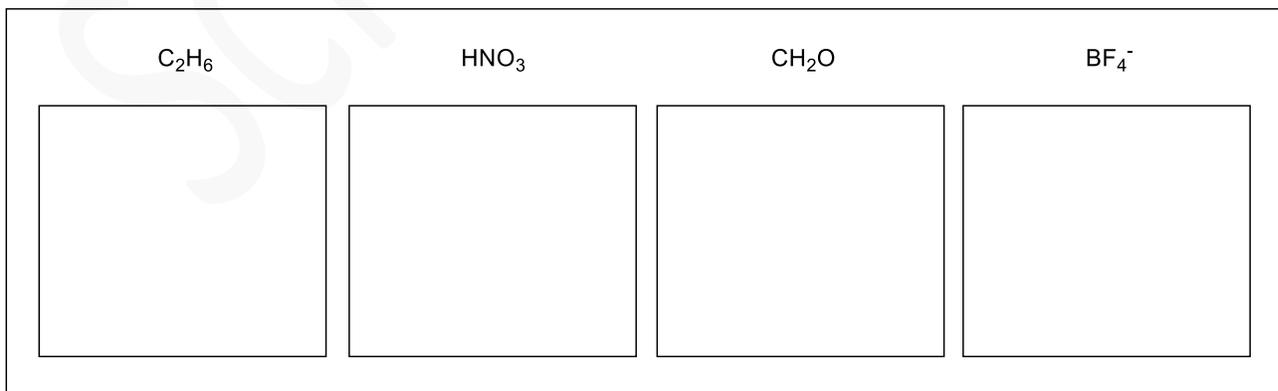
a. Atoms which have fewer than eight valence electrons:

1. Hydrogen only needs two electrons to obtain a full outer shell, and the element can also be stable with zero electrons.
2. Boron and Beryllium can be stable with fewer than 8 electrons: 4 in the case of Beryllium, and 6 in the case of Boron.

b. Atoms which have more than eight valence electrons:

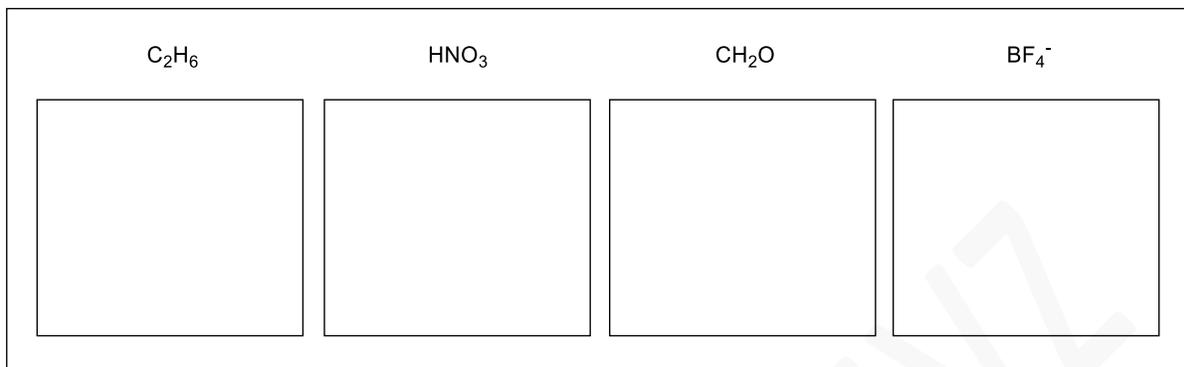
1. Non-metals in Period 3 or higher can exceed the octet rule and maintain more than 8 electrons around their nuclei (ex. Cl, Br, S, P, Ar, Kr, Sn, Sb, Xe).

Example: Determine the Lewis structure for the compounds listed below.

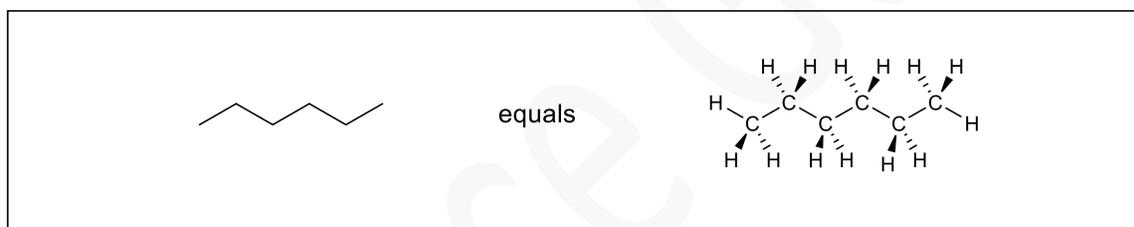


V. Kekulé structures: Drawn like Lewis structures, but omitting the lone pairs.

Example: Determine the Kekulé structures for the following compounds.



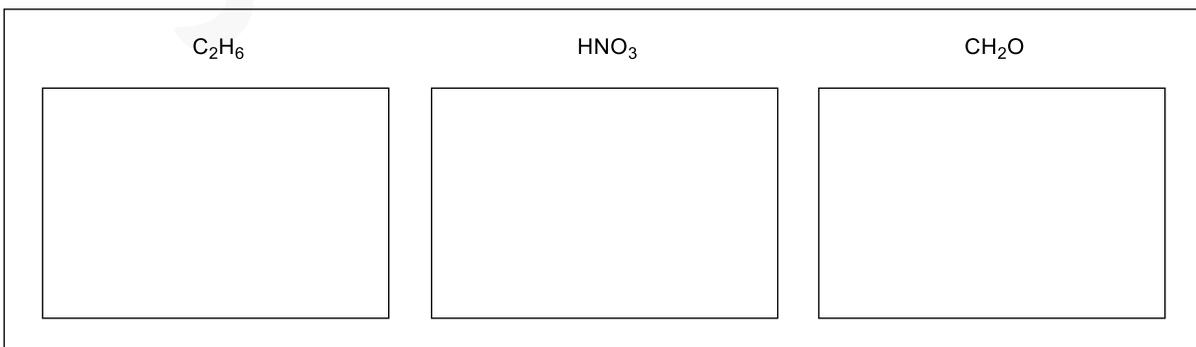
VI. Skeletal Structures (Bond-Line Structures): A method of depicting carbon atoms in a molecule in a quick and concise manner using zig-zag lines. This is the form that you will see most often throughout this course.



a. Understanding Skeletal Structures:

1. Each vertex in a skeletal form equates to a carbon.
2. It is assumed that hydrogen atoms fill the valence of carbon.
3. Remember, neutral carbon **MUST** make four bonds to satisfy the octet rule.
4. Hydrogen atoms attached to carbons are **NEVER** drawn when depicting a molecule in skeletal form.
5. **Always** draw out all non-carbon atoms and any hydrogen atoms attached thereto.
6. Carbocations, carbanions and carbon radicals **ONLY** make 3 bonds.

Example: Draw the skeletal structure of the compounds listed below.

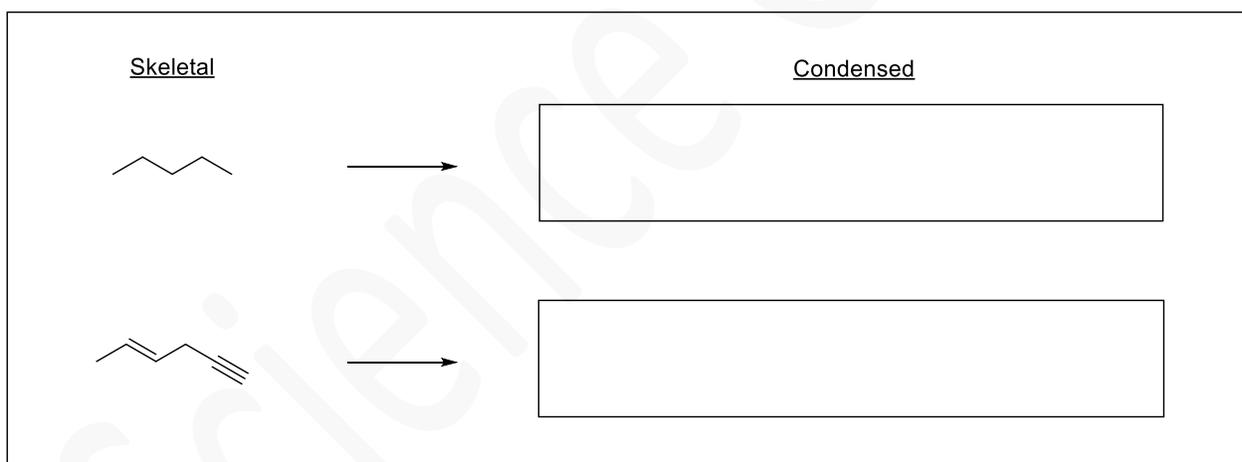


VII. Condensed formulas: Method of depicting an organic compound in which covalent bonds are omitted and atoms bound to a particular carbon are listed next to it (with a subscript for multiple of the same branches).

a. Converting from Skeletal to Condensed Formulas:

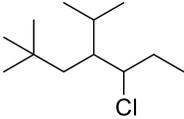
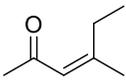
1. Identify a continuous **zig-zag** chain of carbon atoms in the structure that you wish to convert to condensed.
2. Starting from the carbon furthest to the left in your chain and moving right, identify each carbon and the number of hydrogen atoms attached to each carbon.
3. Draw each carbon and its corresponding hydrogen atoms attached in sequence. The hydrogen atoms are typically listed directly to the right of the carbon to which they are attached.
4. 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.
5. Heteroatoms (non-carbon atoms) which are attached to a carbon should be drawn next to the hydrogen atoms which are attached to the heteroatom's attached carbon.

Example: Convert the following skeletal structure into condensed structures.



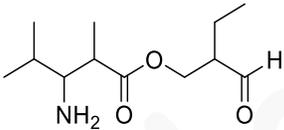
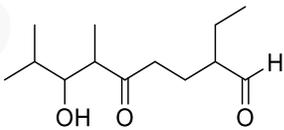
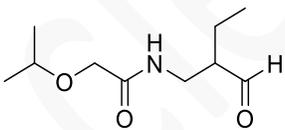
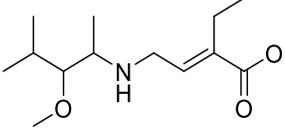
- b. Branching in condensed formulas:** when there are groups of atoms (more than one atom) coming off your continuous chain, these are known as **substituents**.
- c. Substituents will always be placed in parenthesis.** Sometimes you will have branching within substituents and in these cases, you will have to use multiple sets of parentheses.
 1. **Example:** An alcohol group (OH) is a substituent, but a bromine atom (Br) is not.

Example: Convert the following skeletal structures into condensed structures.

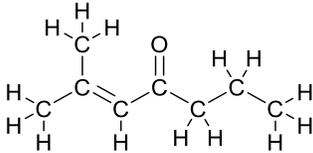
<u>Skeletal</u>	<u>Condensed</u>
	<div style="border: 1px solid black; height: 40px; width: 100%;"></div>
	<div style="border: 1px solid black; height: 40px; width: 100%;"></div>

Example: Match the following condensed formulas to their skeletal structures.

A. $(\text{CH}_3)_2\text{CHCH}(\text{NH}_2)\text{CH}(\text{CH}_3)\text{CO}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHO}$
 B. $(\text{CH}_3)_2\text{CHCH}(\text{OCH}_3)\text{CH}(\text{CH}_3)\text{NHCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CO}_2\text{H}$
 C. $(\text{CH}_3)_2\text{CHOCH}_2\text{CONHCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHO}$
 D. $(\text{CH}_3)_2\text{CHCH}(\text{OH})\text{CH}(\text{CH}_3)\text{COCH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHO}$

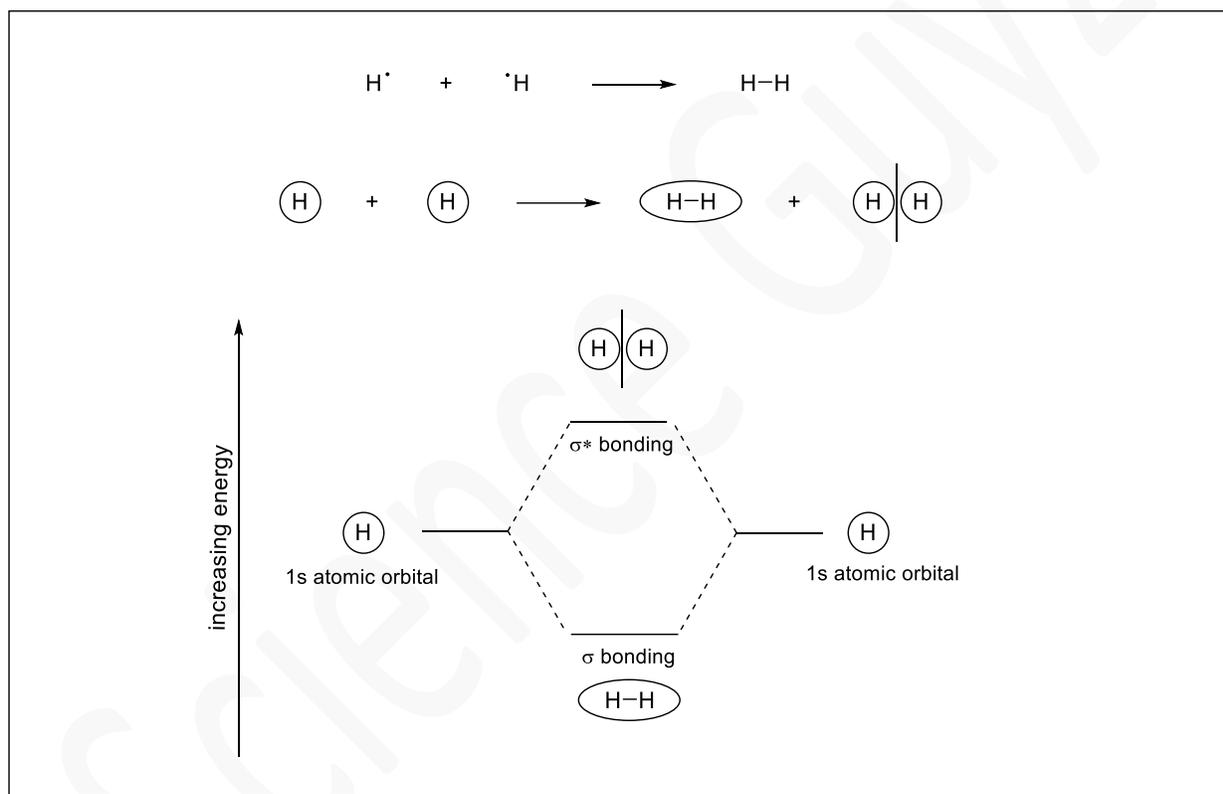
 <div style="border: 1px solid black; width: 40px; height: 20px; display: inline-block; margin-left: 10px;"></div>	 <div style="border: 1px solid black; width: 40px; height: 20px; display: inline-block; margin-left: 10px;"></div>
 <div style="border: 1px solid black; width: 40px; height: 20px; display: inline-block; margin-left: 10px;"></div>	 <div style="border: 1px solid black; width: 40px; height: 20px; display: inline-block; margin-left: 10px;"></div>

Example: Convert the following Kekule structure into condensed structure.

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Molecular Orbital Theory (MO Theory):

- I. **MO Theory** states that covalent bonds form when atomic orbitals combine to create molecular orbitals.
- II. **Atomic orbital:** the volume of space around a nucleus where an electron is likely to be found (surrounds an atom).
- III. **Molecular orbital:** the volume of space around a molecule where an electron is likely to be found (surrounds a molecule).
- IV. When atoms combine to form molecules, the number of orbitals is conserved. For example, when two atomic orbitals are combined, two molecular orbitals are formed: one in higher energy and one in lower energy than the atomic orbitals.



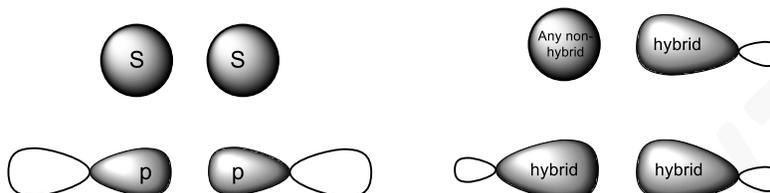
Hybridization:

- I. The combination of different energy atomic orbitals to form new, equal energy hybrid orbitals to create an equal distribution of electron density. Unequal distribution of electrons leads to instability. In Organic Chemistry, we are mostly concerned with sp , sp^2 and sp^3 hybridization.
- II. The theory of hybridization is employed to teach how atoms form chemical bonds and to explain the geometry of atoms within a compound.
- III. Hybridization occurs when an atom is preparing to bond, it is **not** the act of bonding itself. Bonding occurs when orbitals overlap.

Types of Orbital Overlap:

- I. **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.

Examples of Sigma Bonds (σ)



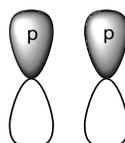
- II. **Sigma Anti-Bonding:** Form when valent orbitals overlap head-on and out-of-phase (opposite shading). **Note:** when the orbitals below overlap head-on a sigma bond is formed and when the shading is opposite, this is known as “anti-bonding”.

Examples of Sigma Anti-Bonds (σ^*)



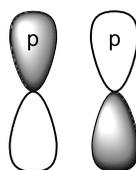
- III. **Pi Bonding:** side-to-side overlap that results in double or triple bonds. Form when valent p-orbitals overlap vertically and in-phase (same shading). Remember, only pure p orbitals can overlap to form a pi bond (hybrid orbitals cannot form pi bonds)!

Examples of Pi-Bonds (π)



- IV. **Pi Anti-Bonding:** Form when valent p orbitals overlap vertically and out-of-phase (opposite shading). **Note:** when the p orbitals below overlap vertically a pi bond is formed and when the shading is opposite, this is known as “anti-bonding”.

Examples of Pi Anti-Bonds (π^*)



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

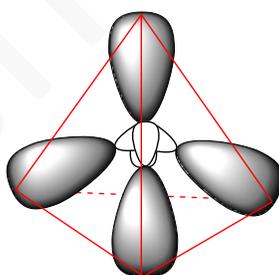
			
σ <input type="checkbox"/>	π <input type="checkbox"/>	σ <input type="checkbox"/>	π <input type="checkbox"/>
σ^* <input type="checkbox"/>	π^* <input type="checkbox"/>	σ^* <input type="checkbox"/>	π^* <input type="checkbox"/>

Hybrid Orbitals:

- I. **sp^3 Hybridization:** Arises upon the mixing of one valent s orbital with three valent p orbitals to form four sp^3 orbitals.



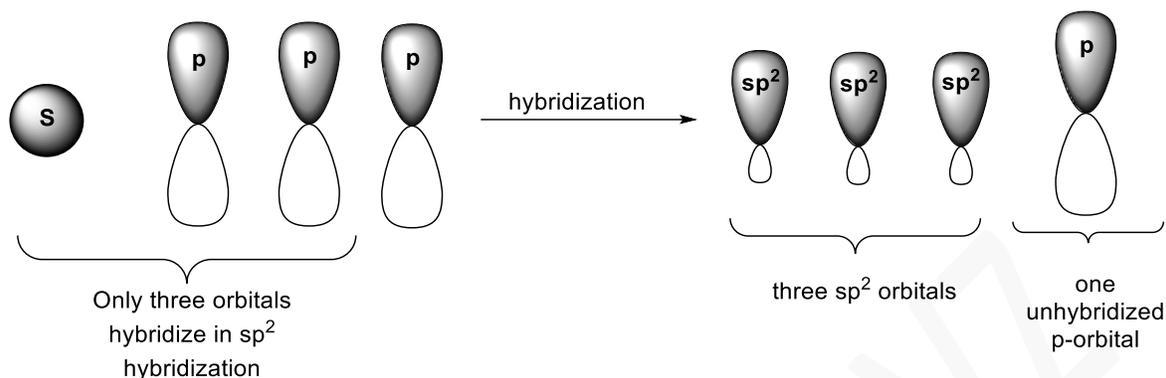
- a. **Geometry of the sp^3 hybridized atom:** Can be understood by imagining that the four sp^3 orbitals formed during sp^3 hybridization are placed around a central point, such that they are as far away from each other as possible. When this is done, a tetrahedron is formed.



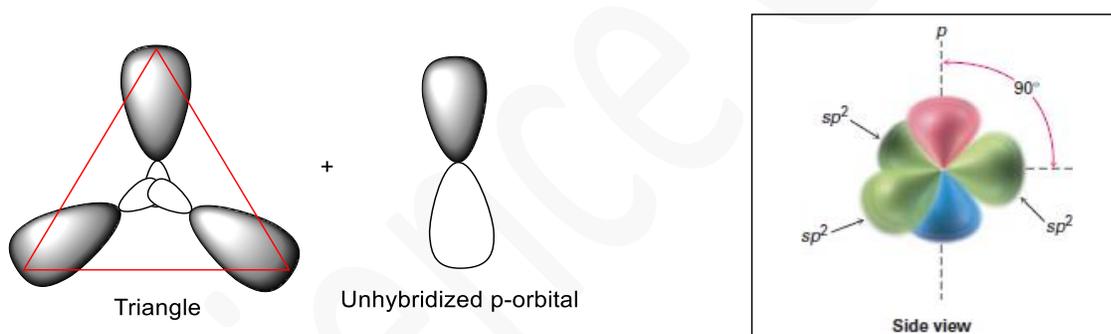
Tetrahedron

- b. **Ideal Bond Angles of the sp^3 hybridized atom:** Correspond to the angles associated with the vertices of a tetrahedron about the center of the tetrahedron. The angles of two vertices of a tetrahedron about the center of the tetrahedron correspond to 109.5° .
- i. **Note:** The bond angles around the sp^3 hybridized atom can deviate from 109.5° depending on whether there are lone pairs of electrons or not. In this class, we are mostly concerned with ideal bond angles.

II. **sp^2 Hybridization:** Arises upon the mixing of one valent s orbital with two valent p orbitals to form three sp^2 orbitals, leaving behind one non-hybridized valent p orbital.



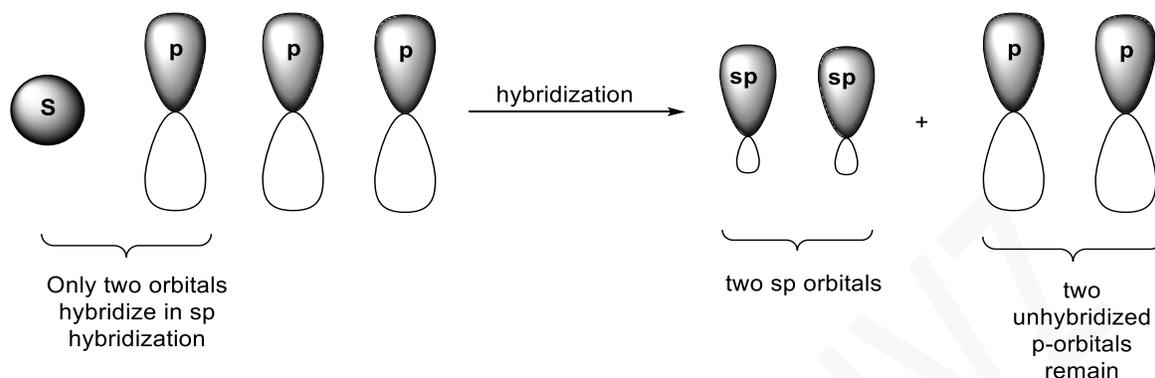
- a. **Geometry of the sp^2 hybridized atom:** Can be understood by imagining that the three sp^2 orbitals formed during sp^2 hybridization are placed around a central point, such that they are as far away from each other as possible. When this is done, a triangle is formed.
- i. **Note:** that when a valent non-hybridized p orbital remains after hybridization, the p orbital must be oriented perpendicular to the plane of the hybrid orbitals.



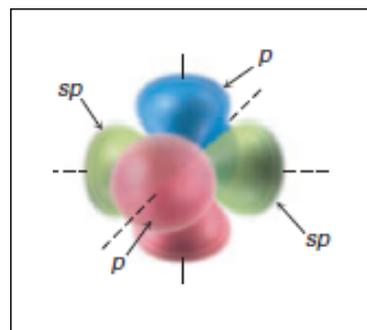
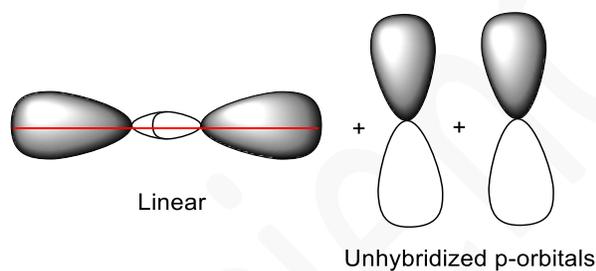
A view of all valent orbitals together after hybridization. Note that the p-orbitals MUST be perpendicular to the hybrid orbitals. P orbitals are not responsible for the geometry of the hybridized atom.

- b. **Ideal Bond Angles of the sp^2 hybridized atom:** Correspond to the angles associated with the vertices of an equilateral triangle about the center of the triangle. The angles of two vertices of a triangle about the center of the triangle correspond to 120° .
- i. **Note:** The bond angles around the sp^2 hybridized atom can deviate from 120° depending on whether there are lone pairs of electrons or not. In this class, we are mostly concerned with ideal bond angles.

III. sp Hybridization: Arises upon the mixing of one valent s orbital with one valent p orbital to form two sp orbitals, leaving behind two non-hybridized valent p orbitals.



- a. **Geometry of the sp hybridized atom:** Can be understood by imagining that the two sp orbitals formed during sp hybridization are placed around a central point, such that they are as far away from each other as possible. When this is done, a line is formed.
- i. **Note:** following sp hybridization, two valent p orbitals remaining. The remaining valent p orbitals must be oriented perpendicular to the plane of the hybrid orbitals.



A view of all valent orbitals together after hybridization. Note that the p-orbitals **MUST** be perpendicular to the hybrid orbitals. P-orbitals are not responsible for the geometry of the hybridized atom.

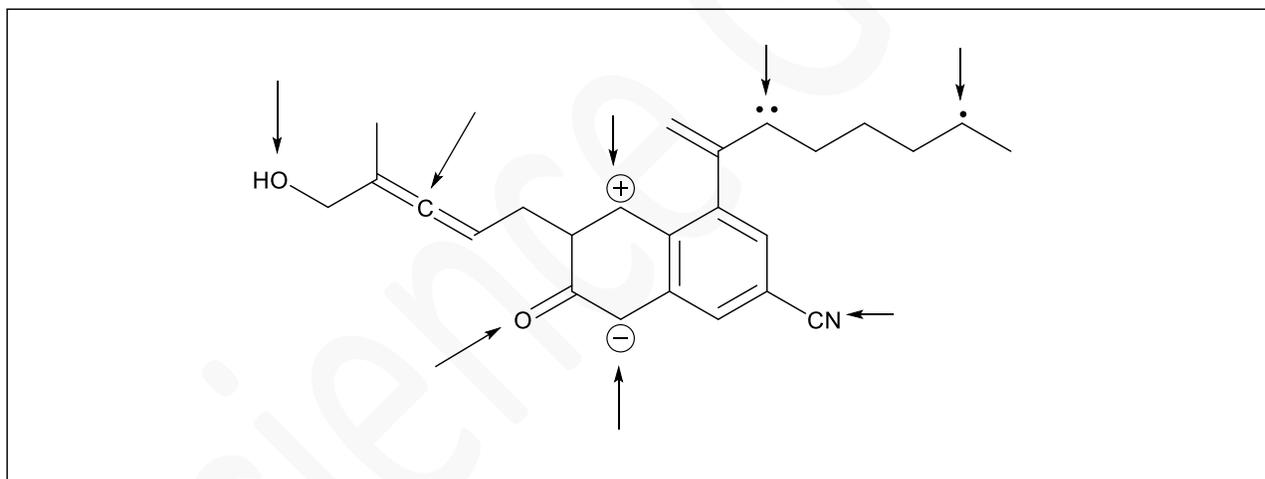
- b. **Ideal Bond Angles of the sp hybridized atom:** The bond angles around a sp hybridized atom correspond to the angles associated with the vertices of a line about the center of the line. The angles of two vertices of a line about the center of the line correspond to 180° .

V. Determining Hybridization of an Atom: Recall from general chemistry that the hybridization of a molecule can be determined by summing the regions of electron density that exist around the atom under analysis. A region of electron density simply refers to where electrons can be found.

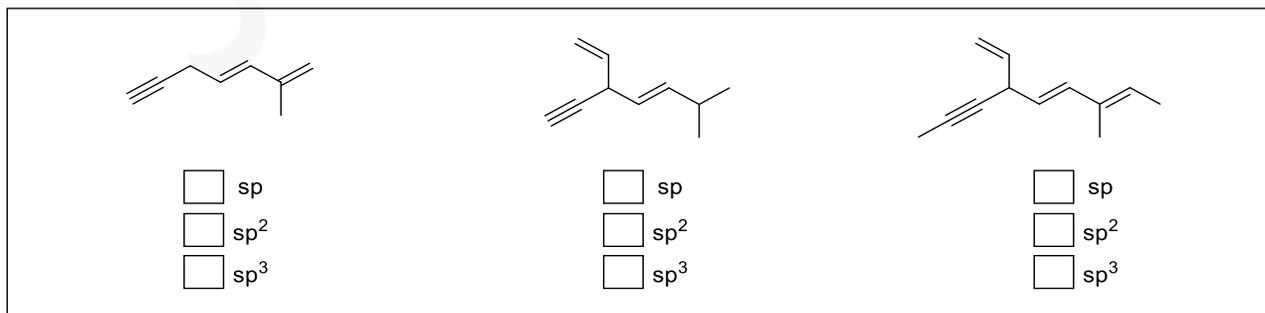
- One region of electron density can be a lone pair, a single bond, a double bond, or a triple bond. Note that single electrons are not counted as a region of electron density.
- After totaling the regions of electron density, the hybridization can be determined using the chart below:

Regions of Electron Density	Hybridization	Electronic Geometry	Ideal Bond Angles
2	sp	Linear	180°
3	sp ²	Trigonal Planar	120°
4	sp ³	Tetrahedral	109.5°

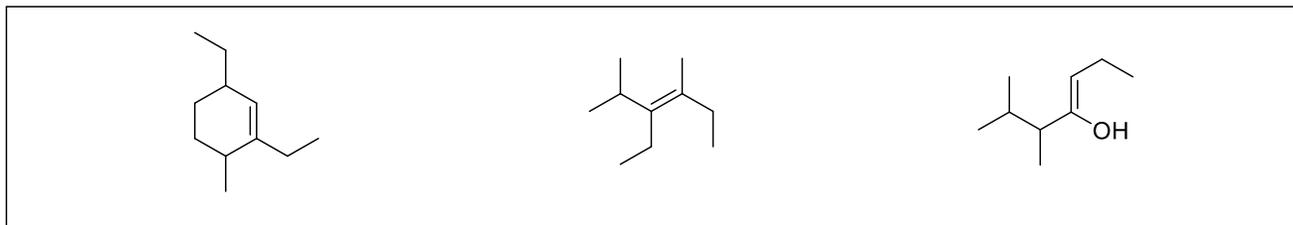
Example: Determine the hybridizations on the atoms indicated below.



Example: Which of the following compounds contains two sp carbons, four sp² carbons, and four sp³ carbons?



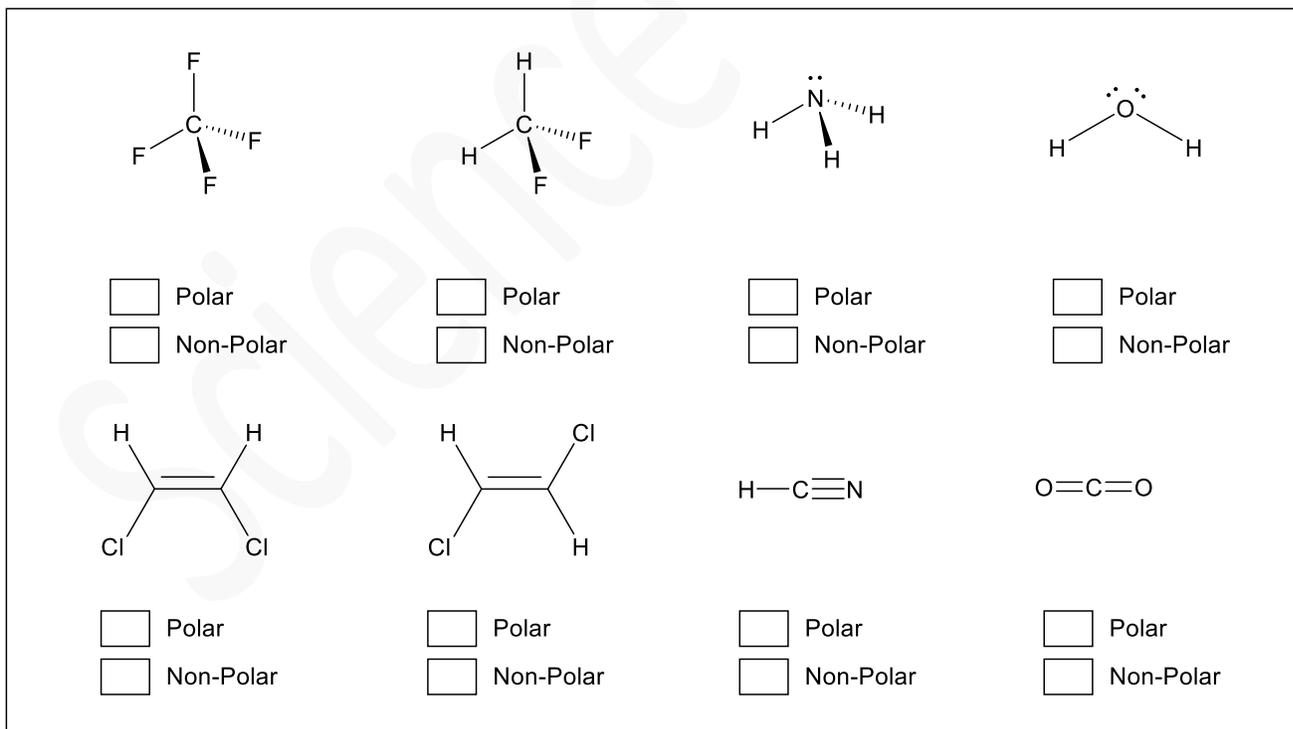
Example: Circle the atoms that lie in the same plane as the sp^2 carbons in the compounds shown below.



Combining Molecular Geometry and Polarity in Polyatomic Molecules:

- I. One must keep molecular geometry in mind when assessing the polarity of more complex molecules. Remember that we draw in 2D but really need to imagine these molecules in 3D to come to the correct answer.
- II. Remember, a polyatomic molecule containing only non-polar bonds is a non-polar molecule.
- III. However, a polyatomic molecule containing polar bonds that are not evenly distributed about the molecules center are polar molecules.
- IV. If a molecule contains polar bonds in equal and opposite directions, then that molecule is non-polar.

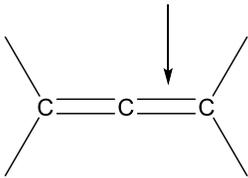
Example: Determine if the molecules shown below are polar or nonpolar.



Determining Which Orbitals Overlap to form an Indicated Bond:

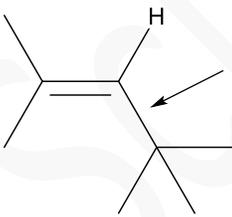
- I. Determine what type of bond is present by looking at the Lewis or line-bond structure of your compound and ask the following: "Is this a single bond, double bond, or triple bond?"
- II. Next determine which orbitals overlap to form the indicated bond.
 - a. Single bond composition: only composed of a sigma bond.
 - b. Double bond composition: composed of one pi bond and one sigma bond.
 - c. Triple bond composition: composed of two pi bonds and one sigma bond.

Example: Describe the bond type and composition of the indicated bond in the structure below.

	<u>Bond Type:</u> <input style="width: 100%; height: 20px;" type="text"/>	<u>General Bond Composition:</u> <input style="width: 100%; height: 20px;" type="text"/>
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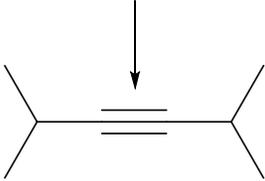
- d. To determine the orbitals that overlap to form a sigma bond, determine the hybridization of the two atoms making the sigma bond. The hybrid orbitals of these atoms will be the orbitals that overlap to make the sigma bond.
- e. Remember: hydrogen atoms do not hybridize. When examining a bond containing hydrogen, the bond will be composed of an s orbital with whatever hybrid orbital is attached to the hydrogen.

Example: Determine the orbitals that overlap to form the sigma bond indicated below.

	<u>Bond Type:</u> <input style="width: 100%; height: 20px;" type="text"/>	<u>Specific Bond Composition:</u> <input style="width: 100%; height: 20px;" type="text"/>
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- f. To determine the orbitals that overlap to form a pi bond, understand that pi bonds will always be composed of pure p orbitals.

Example: Determine which orbitals overlap to form the indicated bond below.



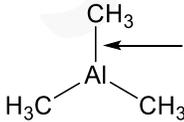
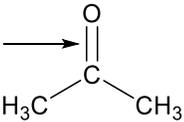
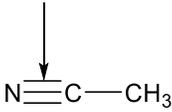
Step 1: Identify bond type and general bond composition.

Step 2: Identify which orbitals overlap to form the sigma bond.

Step 3: Identify which orbitals overlap to form the pi bonds.

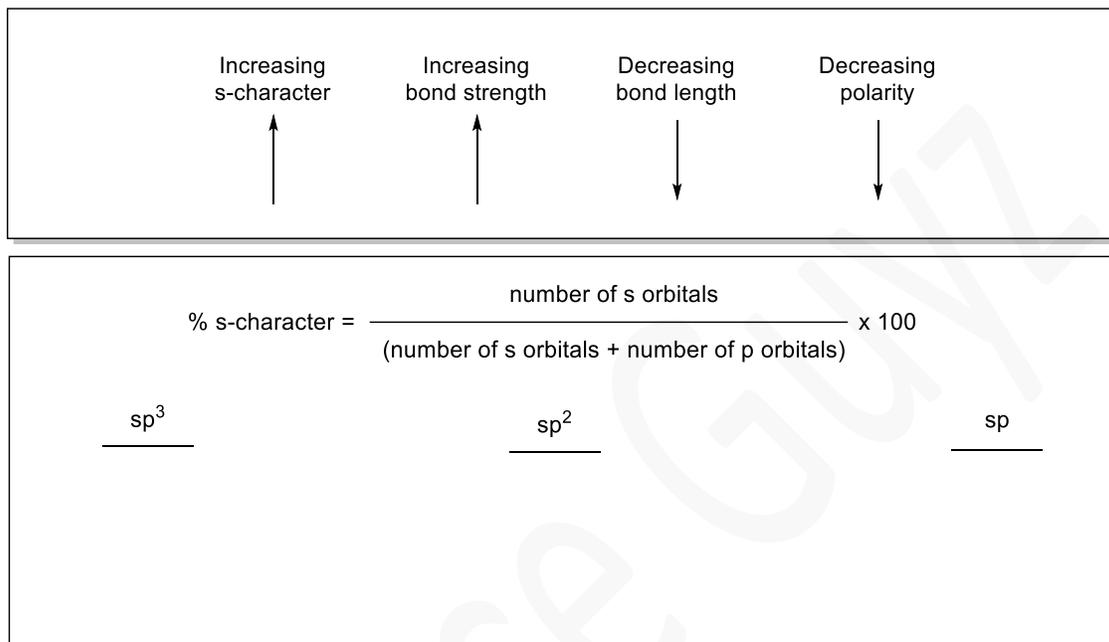
Final answer: Which orbitals overlap to form the indicated bond?

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

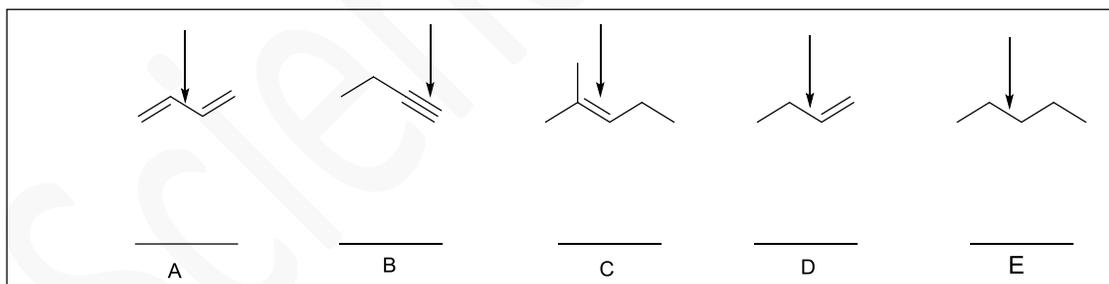
		

Bond Length and Bond Strength:

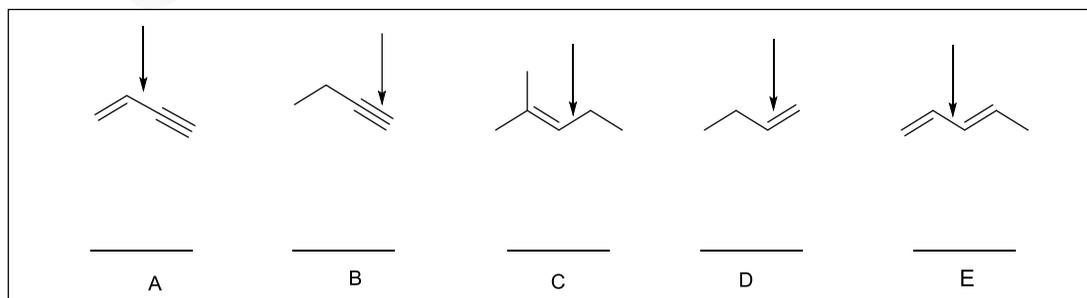
- I. Generally, triple bonds are shorter and stronger than double bonds. Double bonds are shorter and stronger than single bonds. When comparing two bonds of the same type, the shorter/stronger bond will be the bond that has the most s-character.



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

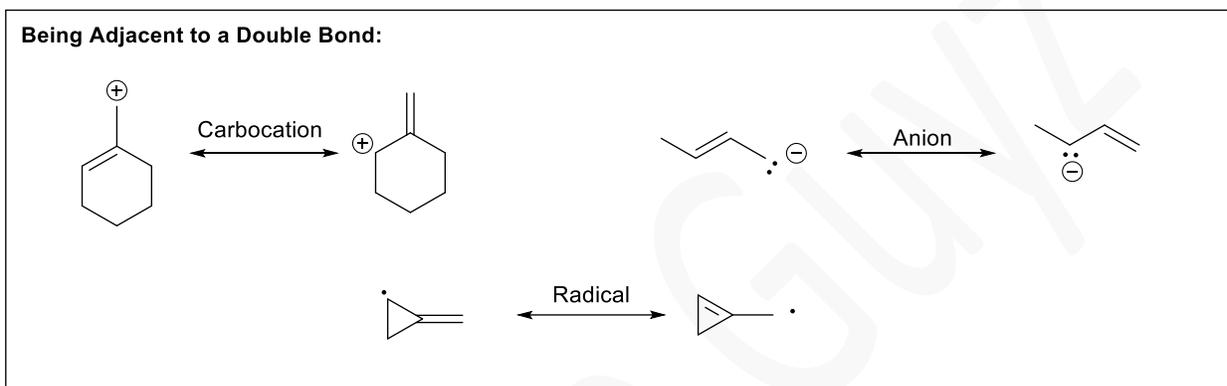


Example: Rank the indicated bonds from weakest to strongest (1 = weakest).

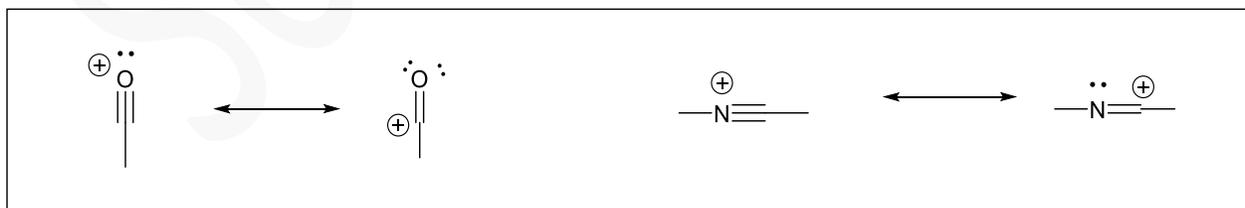


Resonance:

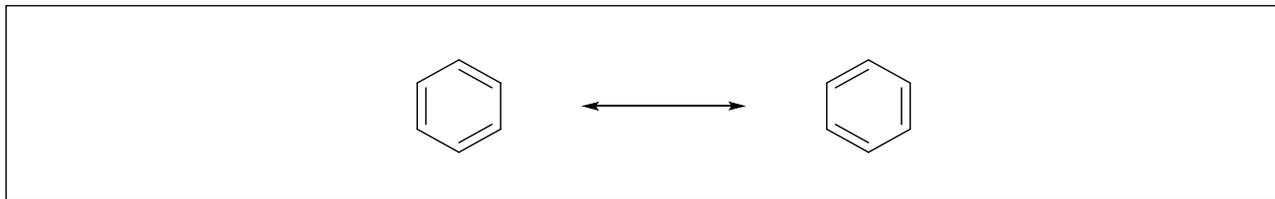
- I. The movement of pi electrons (electrons composing one bond in a double or triple bond) and non-bonding electrons (lone pairs or radicals). **Resonance structures** are identical in terms of molecular structure and energy, but different in the location of electrons.
- II. There are three main types of resonance you will encounter in this course: carbocation, anion, and radical. For a structure to be able to resonate, the carbocation, anion or radical must be adjacent to a pi bond (double or triple bond). Adjacent simply means one atom away from an atom making a double or triple bond (1,3 relationship).



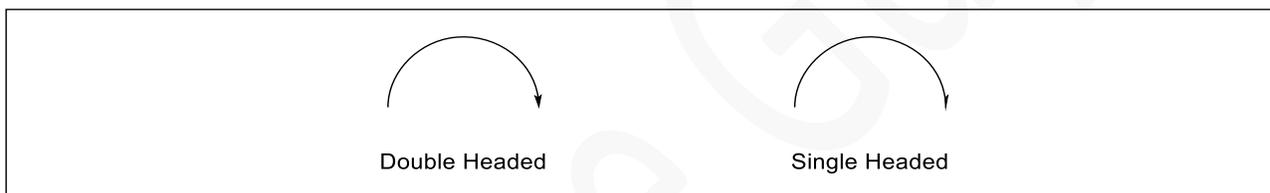
- III. **Rules of Resonance:** When resonating a compound, there are some rules to keep in mind:
 - a. The net charge of the molecule must remain constant. For two forms to be considered resonance forms, the net charge on the compound must remain constant between them.
 - b. Never break sigma (single) bonds, only pi bonds can move.
 - c. Do not violate the octet rule. Be mindful of this rule and its exceptions as you are proposing resonance structures.
- IV. **Some Quirky Exceptions:** When a positively charged oxygen, nitrogen or sulfur is making a double or triple bond, electrons from an ipso double or triple bond can be moved from the bond to the oxygen, nitrogen, or sulfur to create a carbocation and an additional lone pair of electrons on the oxygen, sulfur, or nitrogen.



- a. When you have three alternating double bonds inside of a cyclic ring, you can rearrange the double bonds in the ring creating an additional resonance form.

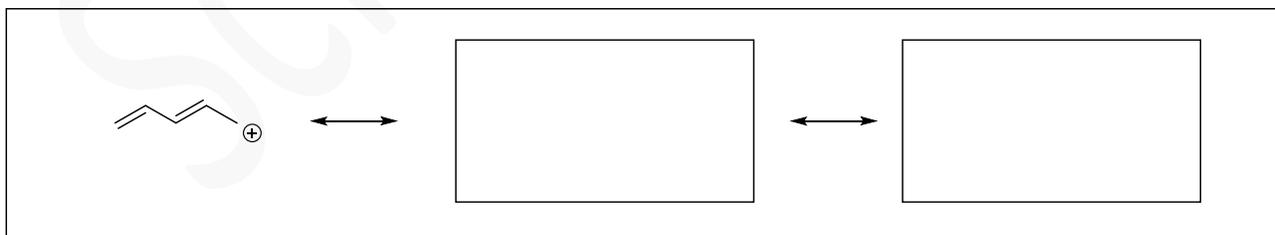


- V. Showing Resonance Using Curved Arrows:** In organic chemistry, we use curly arrows to depict the movement of electrons. Always move electrons by drawing an arrow from the electron source toward the electron accepting atom. The curved arrow should point to the atom which is accepting the electrons.
- Single headed arrows are used to depict the movement of a radical (single electron).
 - Double headed arrows are used to depict the movement of an electron pair.



- VI. Carbocation Resonance:** This type of resonance occurs when there is a "hole" in the molecule where electrons should be.
- Only one arrow is required when resonating a carbocation.
 - Draw an arrow from the electron donating species to the carbocation. This indicates that the carbon will share the electrons donated with the donor species.

Example: Provide all resonance structures for the compound shown below. Use curly arrows to depict electron movement.



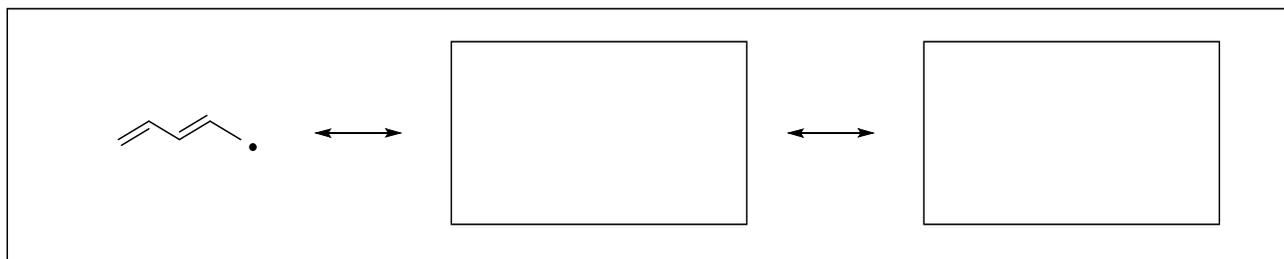
- VII. Anion Resonance:** This type of resonance occurs when you have an excess of electrons that are moving about the molecule. Using Curved Arrows When Resonating an Anion:
- Two curved arrows are required when resonating a carbanion.
 - First, determine the donor species. This will typically be a lone pair of electrons.
 - Next, identify an adjacent atom which is making a double or triple bond. This will be the accepting species.
 - Draw a double headed curved arrow from the donor electrons to the bond of the accepting atom.
 - Next, draw an arrow from a pi-bond of the accepting species to the other adjacent atom of the accepting, creating a new lone pair on the atom adjacent to the accepting atom.

Example: Provide all resonance structures for the compound shown below. Use curly arrows to depict electron movement.

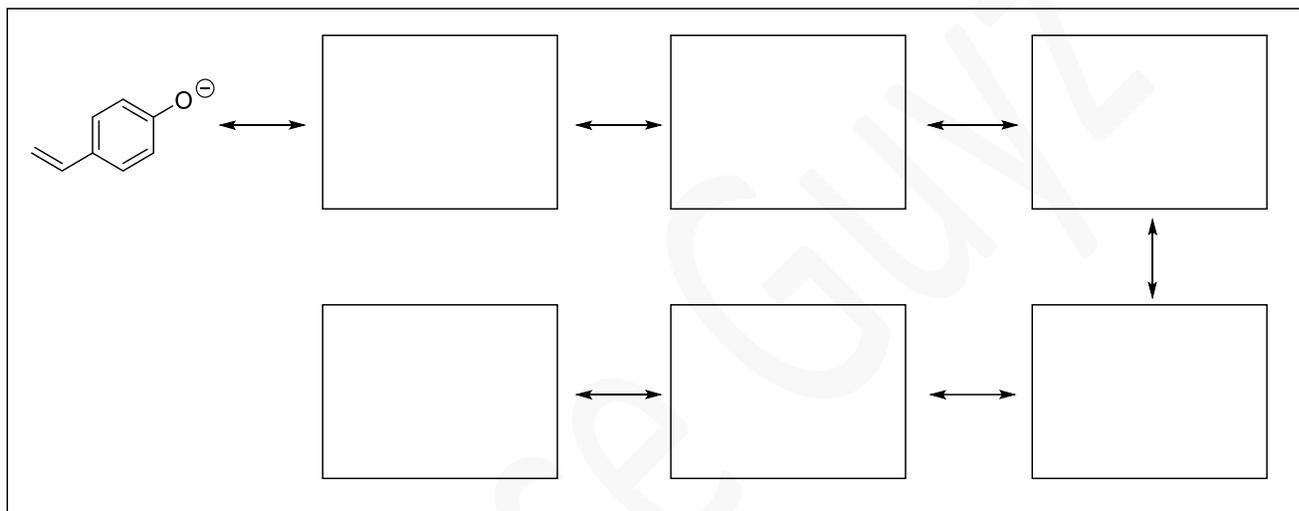
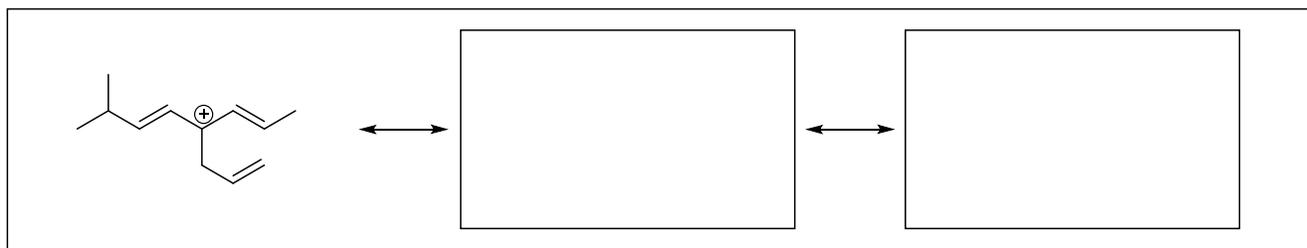


- VIII. Radical Resonance:** This type of resonance occurs when there is a single electron adjacent to a pi bond. Using Resonance When Resonating a Radical:
- Three arrows are required when resonating a radical.
 - First, draw a half arrow from a pi-bond which is adjacent to the radical, to the middle of the bond which connects the atom having the radical to the adjacent atom making the double bond.
 - Second, draw a half arrow from the radical, to the middle of the bond which connects the atom having the radical to the adjacent atom making the double bond, such that it meets up with the half arrow drawn first (this creates a new double bond).
 - Finally, draw a half arrow from the pi-bond adjacent to the radical to the atom at the far end of the pi bond (this will create a new radical).

Example: Provide all resonance forms for the following compound. Use curly arrows to depict electron movement.



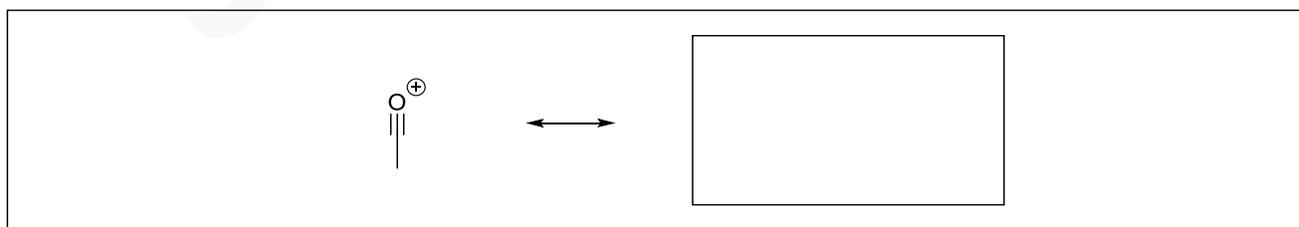
Example: Provide all resonance forms for the structures shown below. Use curly arrows to depict electron movement.



IX. Other Quirky Resonance Issues: Using Curved Arrows When Resonating a ***positively charged O, N, or S*** which directly makes a double or triple bond:

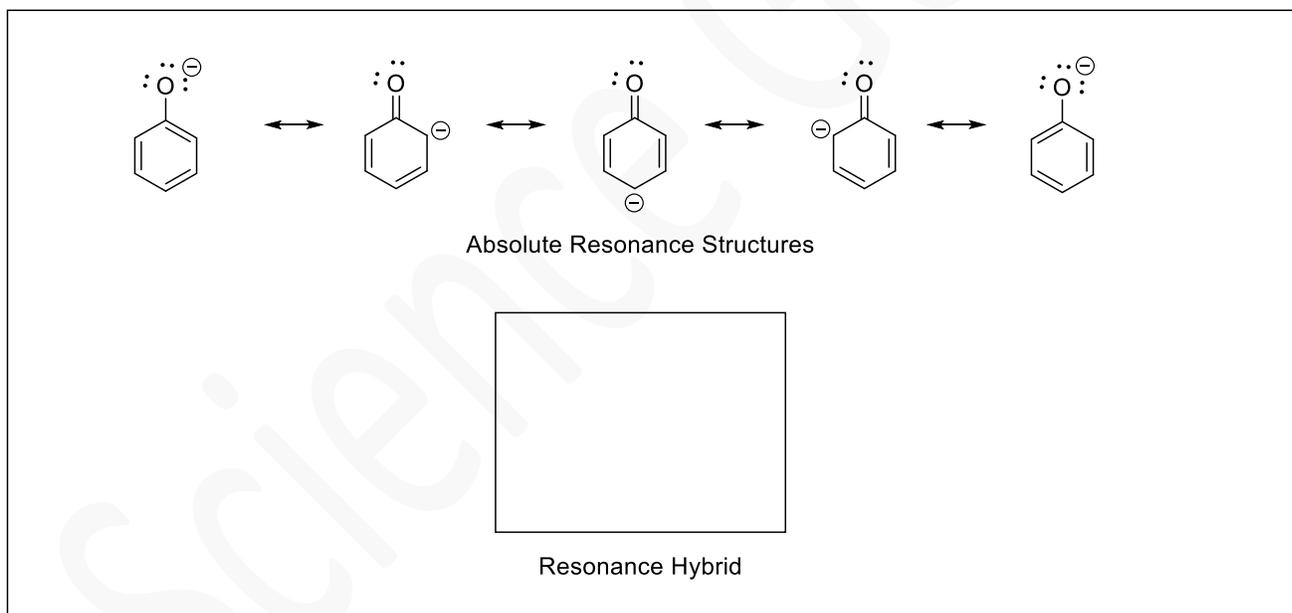
- One arrow is required for this type of resonance.
- Draw a double headed arrow from the electron source (the double/triple bond) back to the positively charged O, N, or S. This will neutralize the charge by adding a lone pair to the atom.
- Remember that O, N, and S must maintain an octet. Carbon however can exist without a full octet (carbon can have 8, 7, or 6 electrons).

Example: Provide all resonance forms for the following compound. Use curly arrows to depict electron movement.



- X. Resonance Hybrid:** The resonance structures that we observed above are absolute resonance structures. In reality, resonance structures exist as a hybrid or an average of all the absolute resonance structures that a molecule can have.
- Drawing Resonance Hybrids: To draw a resonance hybrid, draw a dotted line over the system of pi electrons and/or lone pairs that you moved to create each individual resonance structure.
 - Add a delta symbol (δ) and corresponding charge on each atom that contained a charge in your individual resonance forms.
 - For negative charges δ^-
 - For positive charges δ^+
 - You may be asked to identify the **greatest resonance contributor** out of a set of resonance forms. This simply means to choose the most stable representation of the molecule. This will generally be the contributor/form in which all atoms have an octet, and the negative charge is on the more electronegative atom (or positive charge is on more electropositive atom).

Example: Given the resonance structures below, draw the resonance hybrid. Additionally, circle which resonance form is the most contributing.



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.

$$FC = (\# \text{ val } e^-) - (\# \text{ non-bonding } e^-) - 1/2(\# \text{ bonding } e^-)$$

$$FC = (\# \text{ val } e^-) - (\# \text{ dots}) - (\# \text{ lines})$$

Determining Hybridization

Regions of e^- Density	Hybridization	Geometry	Ideal Bond Angles
2	sp	Linear	180°
3	sp^2	Trigonal Planar	120°
4	sp^3	Tetrahedral	109.5°

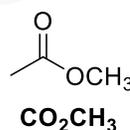
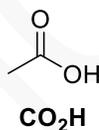
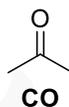
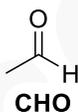
Rules of Resonance:

1. Net charge must remain constant.
2. Never break sigma bonds.
3. Do not violate the octet rule.

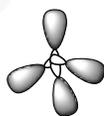
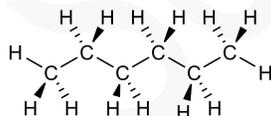
Cation resonance: 1 arrow

Anion resonance: 2 arrows

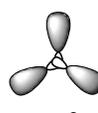
Radical resonance: 3 arrows



equals



sp^3



sp^2



sp

σ : head-to-head overlap, in-phase

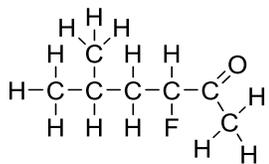
σ^* : head-to-head overlap, out-of-phase

π : vertical overlap, in-phase

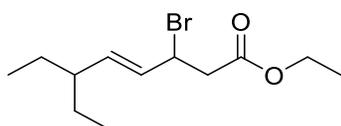
π^* : vertical overlap, out-of-phase

Practice Problems – test your understanding and try these problems out on your own! An answer key will be posted to the Science Guyz website.

1. Convert the following Kekulé structure to condensed structure.



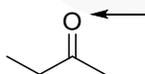
2. Convert the following skeletal structure to condensed structure.



3. Convert the following condensed structure to skeletal structure.



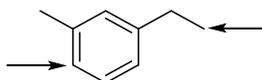
4. Identify the hybridization on the atoms indicated below.



sp

sp²

sp³



sp

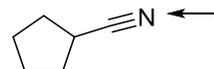
sp²

sp³

sp

sp²

sp³

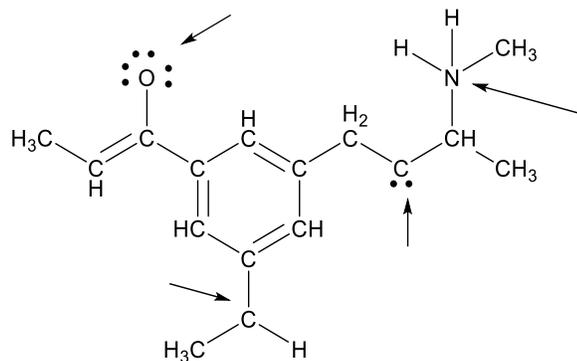


sp

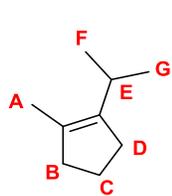
sp²

sp³

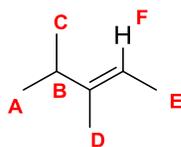
5. Provide the formal charge on the atoms indicated below.



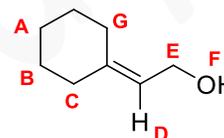
6. Check the boxes to indicate which of the following atoms lay in the same plane as the sp^2 hybridized atoms. Select all that apply.



A	<input type="checkbox"/>
B	<input type="checkbox"/>
C	<input type="checkbox"/>
D	<input type="checkbox"/>
E	<input type="checkbox"/>
F	<input type="checkbox"/>
G	<input type="checkbox"/>

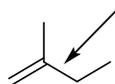


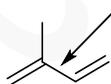
A	<input type="checkbox"/>
B	<input type="checkbox"/>
C	<input type="checkbox"/>
D	<input type="checkbox"/>
E	<input type="checkbox"/>
F	<input type="checkbox"/>

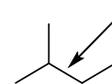


A	<input type="checkbox"/>
B	<input type="checkbox"/>
C	<input type="checkbox"/>
D	<input type="checkbox"/>
E	<input type="checkbox"/>
F	<input type="checkbox"/>
G	<input type="checkbox"/>

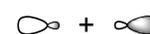
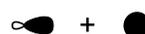
7. Rank the indicated bonds in order of decreasing length (1 = longest).



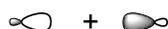




8. Which of the atomic orbital combinations shown below will result in a σ molecular orbital?

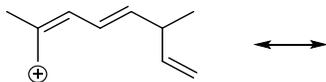


9. Which of the atomic orbital combinations shown below will result in a π^* molecular orbital?

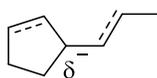
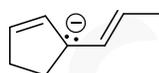


10. Provide all resonance structures and the resonance hybrid for the following compound.

Hybrid



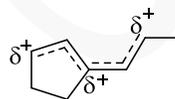
11. Which of the following is the resonance hybrid for the compound below?



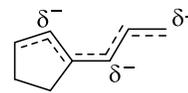
A



B

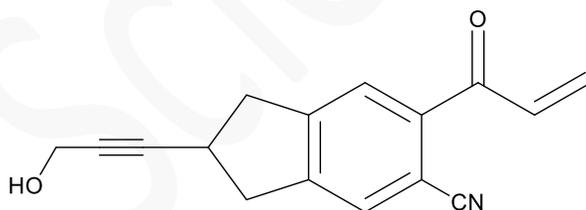


C



D

12. 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.



C H O N

**Sigma
Bonds**

**Pi
Bonds**

**sp hybridized
atoms**

**sp² hybridized
atoms**

**sp³ hybridized
atoms**