



ScienceGuyz

CHEM 2211

Chapter 1: Atomic Structure and Hybridization

CORONA EDITION

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Spring 2021

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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.

The Basics

- An atom is composed of a nucleus surrounded by an electron cloud.
 - The nucleus contains positively charged protons and uncharged neutrons.
 - The electron cloud is composed of negatively charged electrons.
- 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.

Stability

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.

Bonding Between Atoms

- 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.
 - Examples:** NaCl, LiOH, MgCl₂, LiCH₃
- 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.
 - Examples:** HBr, CH₄, NH₃

A Deeper Look into Covalent Bonding: Electronegativity and Polar Bonds

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.

- I. **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

1 H Hydrogen 1.00794																	2 He Helium 4.003														
3 Li Lithium 6.941	4 Be Beryllium 9.012182															5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.00644	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797										
11 Na Sodium 22.989770	12 Mg Magnesium 24.3050															13 Al Aluminum 26.981538	14 Si Silicon 28.0855	15 P Phosphorus 30.973761	16 S Sulfur 32.066	17 Cl Chlorine 35.4527	18 Ar Argon 39.948										
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955910	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938049	26 Fe Iron 55.845	27 Co Cobalt 58.933200	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80														
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.29														
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 La Lanthanum 138.9055	58 Ce Cerium 140.12	59 Pr Praseodymium 140.90768	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.50087	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93487	70 Yb Ytterbium 173.05468	71 Lu Lutetium 174.967	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.96655	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98038	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	90 Th Thorium (232)	91 Pa Protactinium (231)	92 U Uranium (238)	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)															

INCREASING ELECTRONEGATIVITY

- II. **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**.

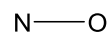
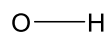
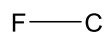
Example: Which of the following bonds are polar?



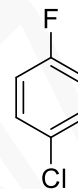
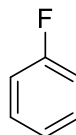
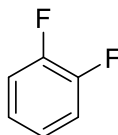
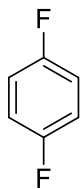
- III. **Dipoles** arise when electrons within a bond are not being shared equivalently. The total dipole moment of a compound is equal to the sum of all individual dipoles. **Dipole moments** refer to the intensity of the dipole and can be calculated by the equation shown below.

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

Example: Using a vector, indicate the dipole in the polar bonds shown below.



Example: Which of the following molecules has the largest dipole? The smallest?



Structural Representations

- I. **Lewis Structures:** structural representation of a molecule/atom/ion that shows all valence electrons and charges.

Steps for drawing Lewis structures:

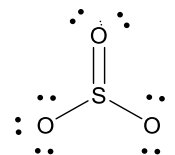
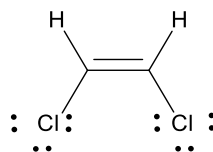
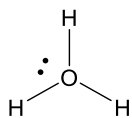
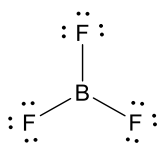
1. **Determine the total number of valence electrons.** Using the molecular formula, sum the total number of valence electrons present in the molecule. For non-neutral compounds (ions), adjust the total count:
 - i. Anions (-): For each negative charge, add one electron
 - ii. Cations (+): For each positive charge, subtract one electron
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 based on the periodic chart, 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. The number of valent electrons present in the connecting atoms can be determined from the periodic chart as well.
 - i. Carbon: 4 bonds, no lone pairs
 - ii. Nitrogen: 3 bonds, 1 lone pair
 - iii. Oxygen: 2 bonds, 2 lone pairs
 - iv. Fluorine: 1 bond, 3 lone pairs
5. **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.
6. **Assign formal charges.** Assign formal charge to each atom in the structure that has a formal charge different than zero.
7. **Choose the favored structure.** Some formulas may yield multiple valid structures. The most favored structure will be the one that minimizes formal charges overall

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 molecules shown below.



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



II. Kekule structures: Drawn similar to Lewis structures, but omitting the lone pairs.

Example: Determine the Kekule structures for the following compounds.



- III. **Skeletal 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.

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.



- IV. **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).

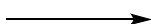
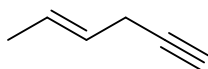
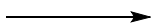
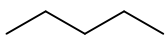
Converting from skeletal to condensed formulas:

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.
 - i. 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.
 - ii. 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.

Skeletal

Condensed



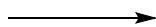
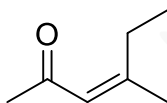
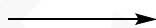
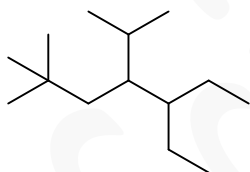
Branching in condensed formulas: when there are groups of atoms (more than one atom) coming off of your continuous chain, these are known as **substituents**.

4. 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.

Example: Convert the following skeletal structures into condensed structures.

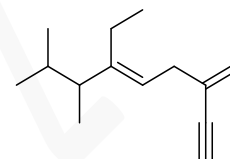
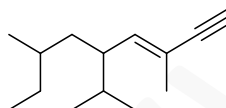
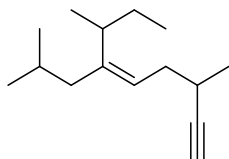
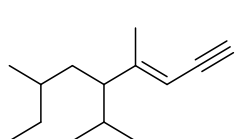
Skeletal

Condensed



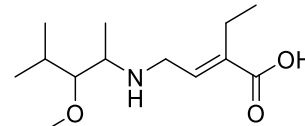
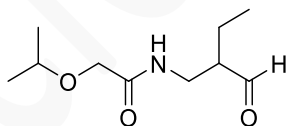
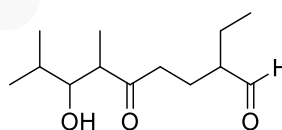
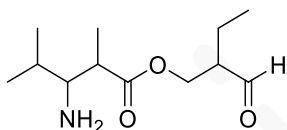
Example: Match the following condensed formulas to their skeletal structures.

- A. $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}(\text{CH}_3)_2)\text{CHC}(\text{CH}_3)\text{CCH}$
- B. $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3)\text{CHCH}_2\text{CH}(\text{CCH})\text{CH}_3$
- C. $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}(\text{CH}_3)_2)\text{C}(\text{CH}_3)\text{CHCCH}$
- D. $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{C}(\text{CH}_2\text{CH}_3)\text{CHCH}_2\text{C}(\text{CCH})\text{CH}_2$

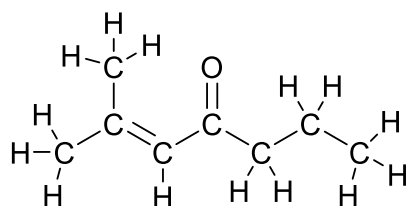


Example: Match the following condensed formulas to their skeletal structures.

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



Example: Convert the following Kekule structure into condensed structure.

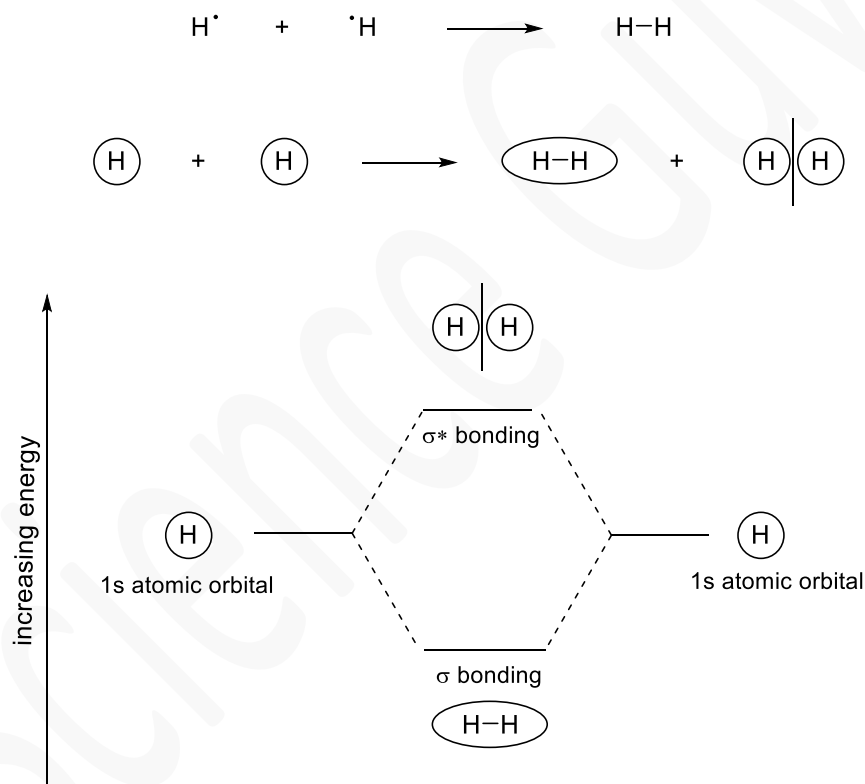


Molecular Orbital Theory (MO Theory): Covalent bonds form when atomic orbitals combine to create molecular orbitals.

- Atomic orbital: the volume of space around a nucleus where an electron is likely to be found (surrounds an atom)
- Molecular orbital: the volume of space around a molecule where an electron is likely to be found (surrounds a molecule)

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.

Example:



Hybridization: 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.

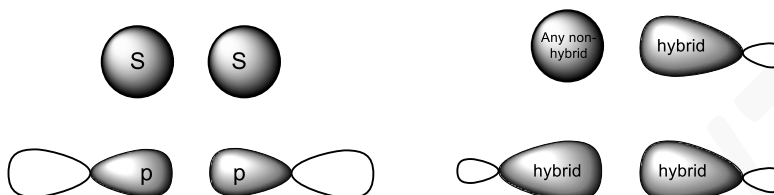
In Organic Chemistry, the theory of hybridization is employed in order to teach how atoms form chemical bonds and to explain the geometry of atoms within a compound.

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 ()



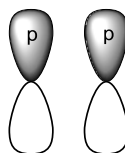
- II. **Sigma anti-bonding:** Form when valent orbitals overlap head-on and out-of-phase (opposite shading). Note: when the orbitals below overlap head-on a sigma bond is formed and when the shading is opposite, this is known as “anti-bonding”.

Examples of Sigma Anti-Bonds (*)



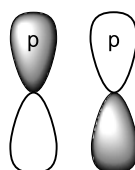
- III. **Pi bonding:** side-to-side overlap that results in double or triple bonds. Form when valent p orbitals overlap vertically and in-phase (same shading). Remember, only pure p orbitals can overlap to form a pi bond! (hybrid orbitals cannot form pi bonds)

Examples of Pi-Bonds ()

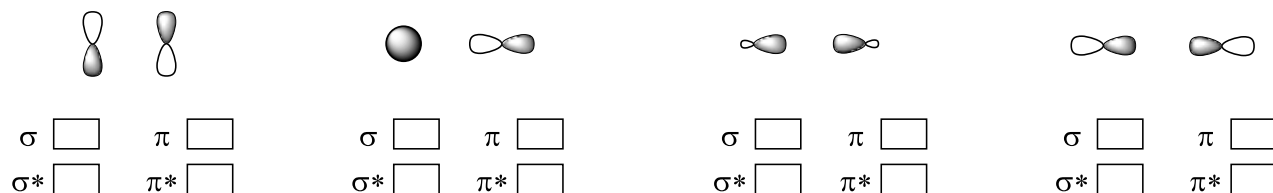


- IV. **Pi anti-bonding:** Form when valent p orbitals overlap vertically and out-of-phase (opposite shading). Note: when the p orbitals below overlap vertically a pi bond is formed and when the shading is opposite, this is known as “anti-bonding”.

Examples of Pi Anti-Bonds (*)



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

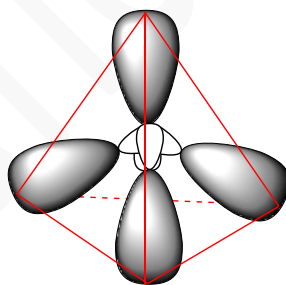


Hybrid Orbitals: sp^3 hybridization

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



- II. **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.

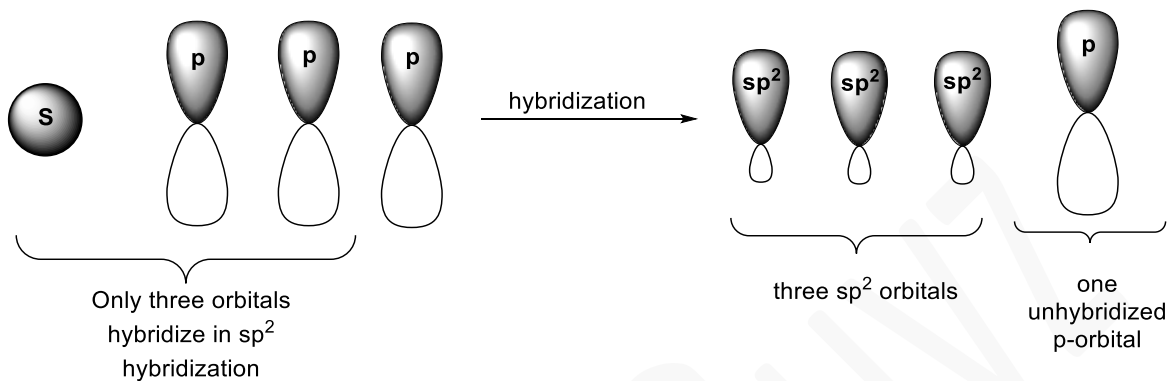


Tetrahedron

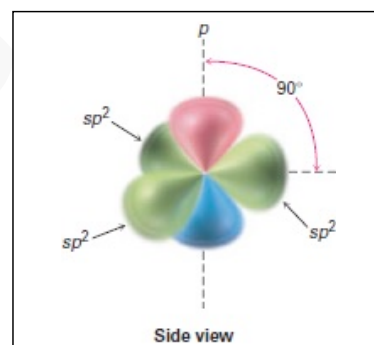
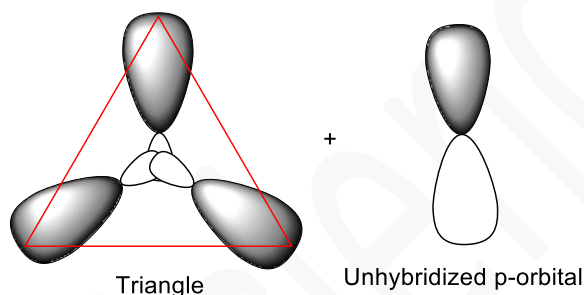
- III. **Ideal Bond Angles of the sp^3 hybridized atom:** Correspond to the angles associated with the vertices of a tetrahedron about the center of the tetrahedron. The angles of two vertices of a tetrahedron about the center of the tetrahedron correspond to 109.5 degrees. Note: The bond angles around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

Hybrid Orbitals: sp^2 hybridization

- I. 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.



- II. **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.
- a. 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.

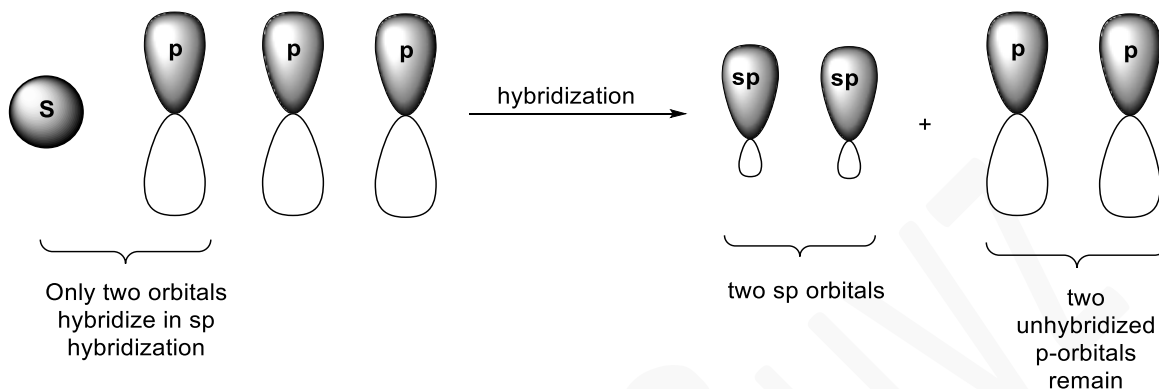


A view of all valent orbitals together after hybridization. Note that the p-orbitals MUST be perpendicular to the hybrid orbitals. P orbitals are not responsible for the geometry of the hybridized atom.

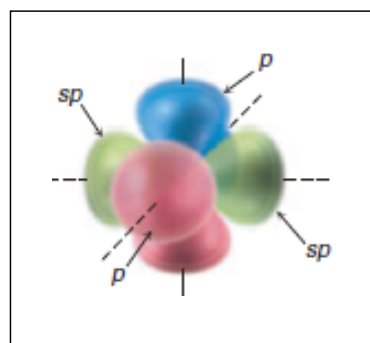
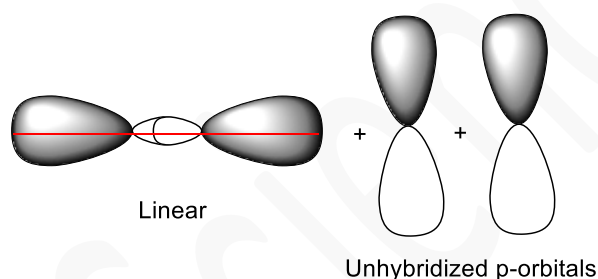
- III. **Ideal Bond Angles of the sp^2 hybridized atom:** Correspond to the angles associated with the vertices of an equilateral triangle about the center of the triangle. The angles of two vertices of a triangle about the center of the triangle correspond to 120 degrees.
- a. Note: The bond angles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

Hybrid Orbitals: sp hybridization

- I. 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.



- II. **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.
- a. Note that 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.

- III. **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 degrees.

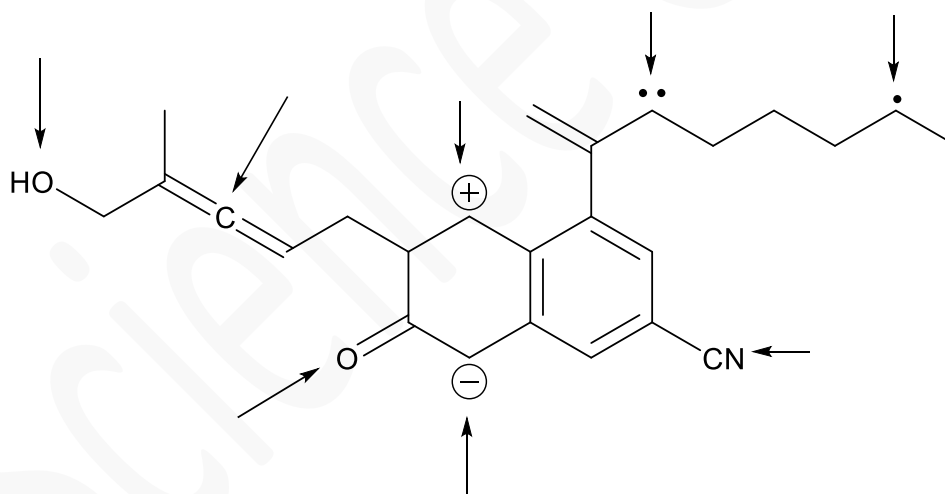
Determining hybridization by looking at an atom in a molecule:

Recall from General Chemistry that hybridization can be determined for any atom by determining the number of regions of electron density that exist around the atom under analysis. Remember that a region of electron density simply refers to where electrons can be found.

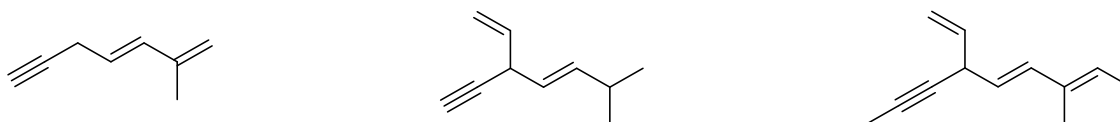
- One region of electron density can be a lone pair of electrons, a single bond, a double bond or a triple bond
 - NOTE! SINGLE ELECTRONS (radicals) ARE NOT COUNTED AS A REGION OF ELECTRON DENSITY. They are just too small and insignificant (sorry, radicals!)
- After counting the number of regions of electron density, one can determine the hybridization of an atom using the chart below.

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

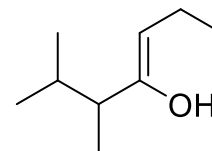
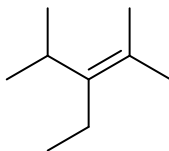
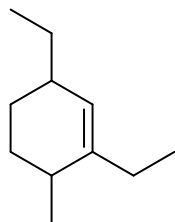
Example: Determine the hybridizations on the atoms indicated below.



Example: Which of the following compounds contains two sp carbons, four sp^2 carbons, and four sp^3 carbons?



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



Combining Molecular Geometry and Polarity in Polyatomic Molecules

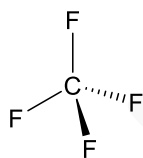
One must keep molecular geometry in mind when assessing the polarity of more complex molecules. Remember that we draw in 2D but really need to imagine these molecules in 3D to come to the correct answer.

Remember, a polyatomic molecule containing only non-polar bonds is a non-polar molecule.

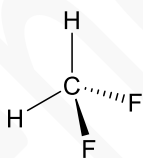
However, a polyatomic molecule containing polar bonds that are not evenly distributed about the molecule's center are polar molecules.

If a molecule contains polar bonds in equal and opposite directions, then that molecule is non-polar.

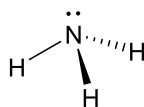
Example: Determine if the molecules shown below are polar or nonpolar.



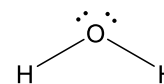
☐ Polar
☐ Non-Polar



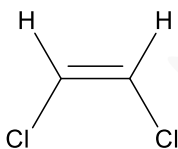
☐ Polar
☐ Non-Polar



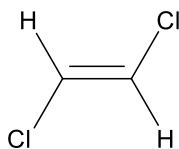
☐ Polar
☐ Non-Polar



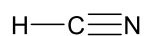
☐ Polar
☐ Non-Polar



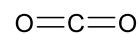
☐ Polar
☐ Non-Polar



☐ Polar
☐ Non-Polar



☐ Polar
☐ Non-Polar



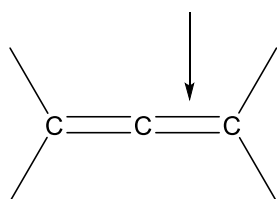
☐ Polar
☐ Non-Polar

Determining which orbitals overlap to form an indicated bond

The process:

1. 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?"
2. 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.

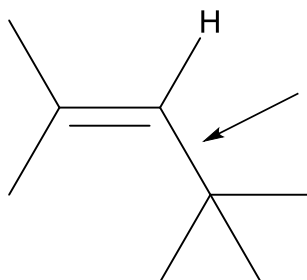


Bond Type:

Bond Composition:

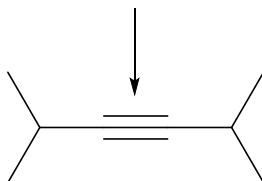
3. To determine the orbitals that overlap to form a sigma bond, determine the hybridization of the two atoms making the sigma bond. The hybrid orbitals of these atoms will be the orbitals that overlap to make the sigma bond.
 - a. Remember: hydrogen atoms do not hybridize. When examining a bond containing 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.



4. 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.



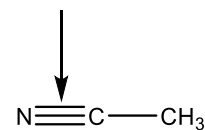
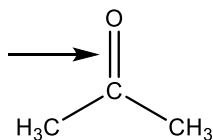
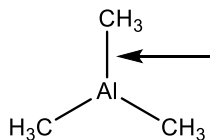
Step 1: Identify bond type and bond composition.

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

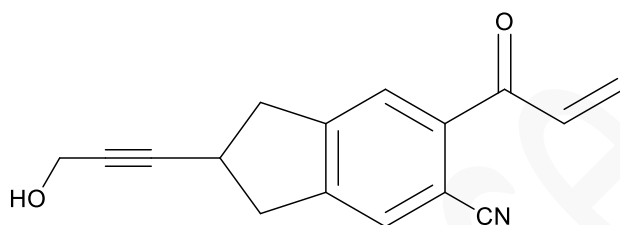
Step 3: Identify which orbitals overlap to form the pi bonds.

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

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



Example: 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

sp^2 hybridized
atoms

sp^3 hybridized
atoms

Bond Length and 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



Decreasing
polarity



To determine the percent s character of each atom making the bond, use the equation below.

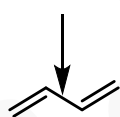
$$\frac{\text{number of } s \text{ orbitals}}{(\text{number of } s \text{ orbitals} + \text{number of } p \text{ orbitals})} \times 100 = \text{percent } s \text{ character}$$

sp^3

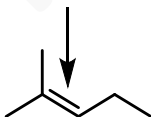
sp^2

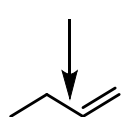
sp

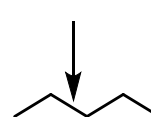
Example: Rank the indicated bonds from longest to shortest. (1 = longest)



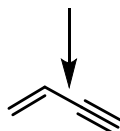


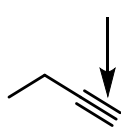


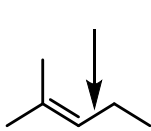


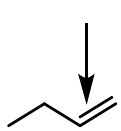


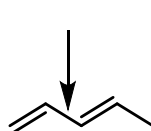
Example: Rank the indicated bonds from weakest to strongest. (1 = weakest)







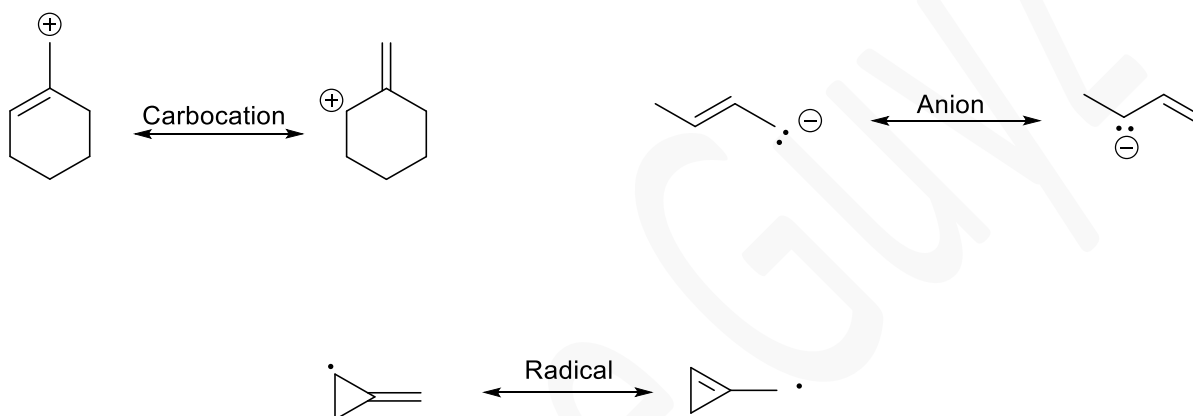




Resonance

Resonance is 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.

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.



Rules of Resonance:

- 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 can move.
- Do not violate the octet rule. Be mindful of this rule and its exceptions as you are proposing resonance structures.
 - Octet rule exceptions:
 - Compounds where an atom has fewer than eight valence electrons:
 - *Hydrogen*: Hydrogen only needs two electrons to obtain a full outer shell, and the element can also be stable with zero electrons.
 - *Boron and Beryllium*: these two elements can be stable with fewer than 8 electrons; 4 in the case of Beryllium, and 6 in the case of Boron.
 - Atoms which have more than eight valent electrons:
 - *Non-Metals in Period 3 or Higher*: these elements can exceed the octet rule and maintain more than 8 electrons around their nuclei.
 - Common Examples: Chlorine, Sulfur, Phosphorus, Bromine Argon, Krypton, Tin, Antimony and Xenon

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. This is favorable because it takes the positive charge off the more electronegative atom.



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.

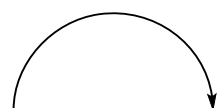


Showing Resonance Using Curved Arrows

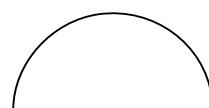
In organic chemistry, we use curly arrows to depict the movement of electrons. Always move electrons by drawing an arrow from the electron source toward the electron accepting atom. The curved arrow should point to the atom which is accepting the electrons.

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.



Double Headed



Single Headed

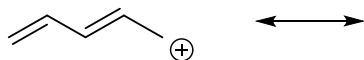
Carbocation Resonance

This type of resonance occurs when there is a “hole” in the molecule where electrons should be.

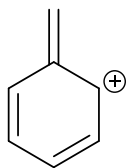
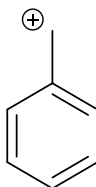
Using Curved Arrows When Resonating a Carbocation:

- 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.

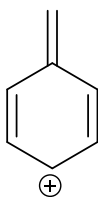
Example: Provide all resonance structures for the compound shown below. Use curly arrows to depict electron movement.



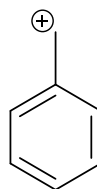
Example: Which of the following structures is not a resonance form of the compound shown below? Select all that apply.



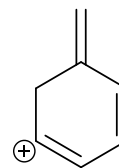
A



B



C



D

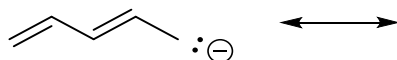
Anion Resonance

This type of resonance occurs when you have an excess of electrons that are moving about the molecule.

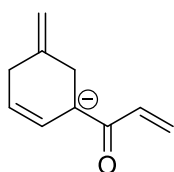
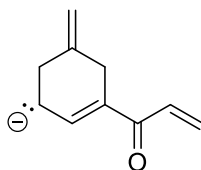
Using Curved Arrows When Resonating an Anion:

- 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.

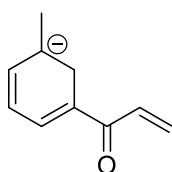
Example: Provide all resonance structures for the compound shown below. Use curly arrows to depict electron movement.



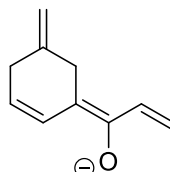
Example: Which of the following structures is not a resonance form of the compound shown below? Select all that apply.



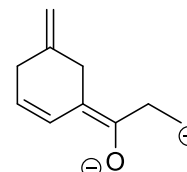
A



B



C



D

Radical Resonance

This type of resonance occurs when there is a single electron adjacent to a pi bond.

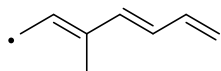
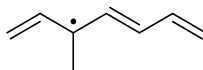
Using Resonance When Resonating a Radical:

- 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).

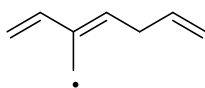
Example: Provide all resonance forms for the following compound. Use curvy arrows to depict electron movement.



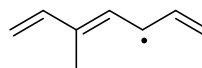
Example: Which of the following structures is not a resonance form of the compound shown below? Select all that apply.



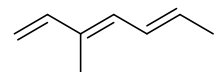
A



B



C



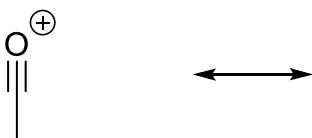
D

Quirky Resonance

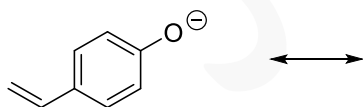
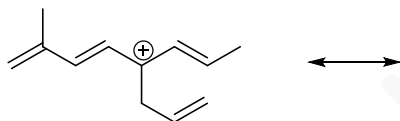
Using Curved Arrows When Resonating a **positively charged O, N, or S** which directly makes a double or triple bond:

- 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.



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



The Resonance Hybrid

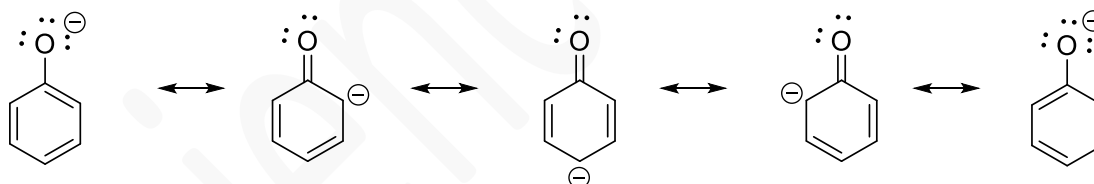
The resonance structures that we observed above are absolute resonance structures. In reality, resonance structures exist as a hybrid or an average of all the absolute resonance structures that a molecule can have.

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.



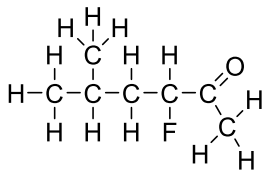
Absolute Resonance Structures



Resonance Hybrid

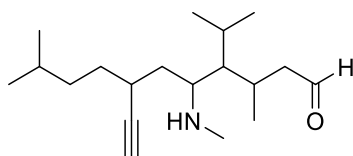
Practice Problems – test your understanding and try these problems out on your own! An answer key will be posted to the ScienceGuyz website.

1. Which of the following condensed formulas corresponds to the Kekule structure shown below?

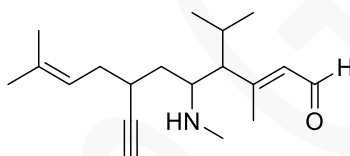


- A. $\text{CH}_3\text{CH}(\text{CH}_3)\text{CHCH}(\text{F})\text{COCH}_3$
 B. $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{F})\text{CHOCH}_3$
 C. $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{F})\text{COCH}_3$
 D. $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{F})\text{COCH}_3$

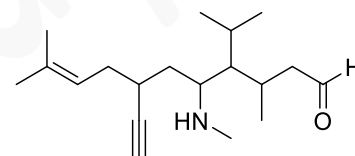
2. Which of the following skeletal structures matches the condensed formula shown below?



A

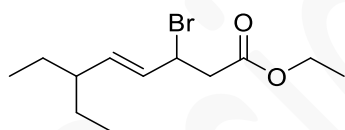


B



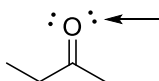
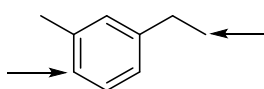
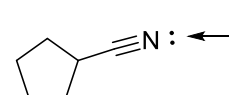
C

3. Which of the following condensed formulas corresponds to the skeletal structure shown below?

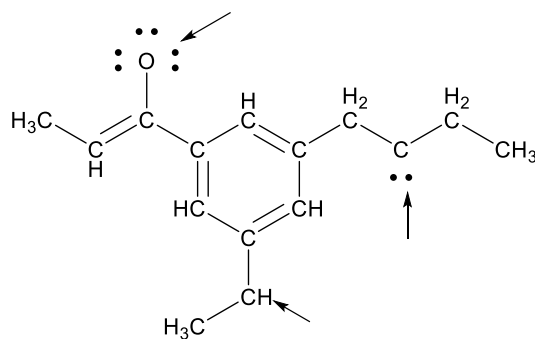


- A. $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}(\text{Br})\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3$
 B. $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHCHCH}(\text{Br})\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3$
 C. $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHCHCH}_2(\text{Br})\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3$
 D. $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_2\text{CH}_3)\text{CHCHCH}(\text{Br})\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3$

4. Identify the hybridization on the atoms indicated below.

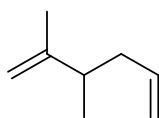
sp ☐sp² ☐sp³ ☐sp ☐sp² ☐sp³ ☐sp ☐sp² ☐sp³ ☐sp ☐sp² ☐sp³ ☐

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

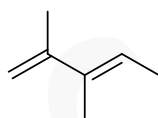


6. Which of the following structures contains 3 sp^3 and 4 sp^2 atoms?

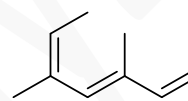
a.



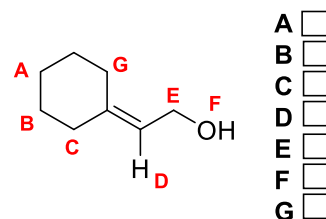
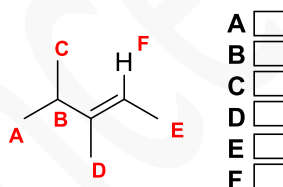
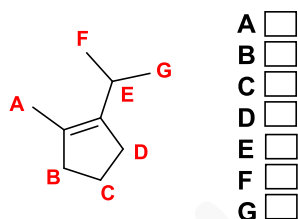
b.



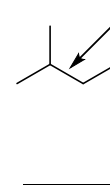
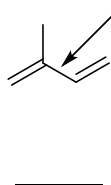
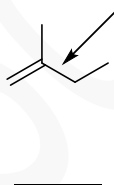
c.



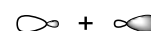
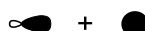
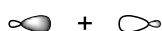
7. Check the boxes to indicate which of the following atoms lay in the same plane as the sp^2 hybridized atoms. Select all that apply.



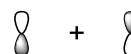
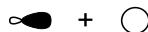
8. Rank the indicated bonds in order of decreasing length (1 = longest).



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

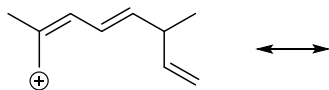


10. Which of the atomic orbital combinations shown below will result in a π^* molecular orbital?

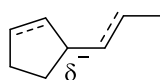
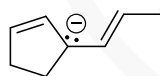


11. Provide all resonance structures and the resonance hybrid for the following compound.

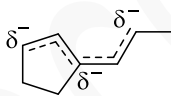
Hybrid



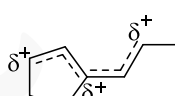
12. Which of the following is the resonance hybrid for the compound below?



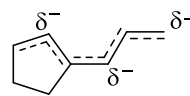
A



B



C



D

13. Which of the following represents correct product formation and electron movement, using curved arrows, for the resonating compounds shown below?

